

10/089964

=> s l1 sss full

FULL SEARCH INITIATED 11:56:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1286 TO ITERATE

100.0% PROCESSED 1286 ITERATIONS
SEARCH TIME: 00.00.01

154 ANSWERS

L3 154 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
157.35	157.56

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:56:26 ON 14 JUL 2003
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FILE LAST UPDATED: 13 Jul 2003 (20030713/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 6 L3

=> d l4 1-6 bib abs hitstr

10/089964

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS
AN 2002:793614 CAPLUS
DN 137:310935
TI Preparation of piperazine derivatives as tachykinin antagonists
IN Pentassuglia, Giorgio
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002081461	A1	20021017	WO 2002-GB1602	20020405
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI	GB 2001-8594	A	20010405		
OS	MARPAT 137:310935				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to piperazine derivs. I [R, R1 = halogen, C1-4-alkyl; R2 = H, C1-4-alkyl; n, m = 1, 2] and pharmaceutically acceptable salts and solvates thereof, to process for their prepn., to pharmaceutical compns. contg. them and to their medical use. The invention also relates to a process: (a) for the prepn. of I, which comprises prepn. via redn. of ketopiperazines II (Ra = H, N-protecting group) with a suitable reducing agent; or (b) for the prepn. of I, which comprises the reaction of phenylpiperazines III (Ra = N-protecting group) with triphosgene and an org. base, followed by addn. of benzylzmines IV; each followed, where necessary or desired by one or more of the following: (i) removal of the nitrogen protecting group; (ii) isolation of the compd. as a salt or solvate thereof; (iii) sepn. of I or its derivs. into the enantiomers thereof. Thus, piperazinyurea V was prepd. from (S)-3-(4-Fluoro-2-methylphenyl)piperazin-2-one via carbonylation with triphosgene in CH2Cl2 contg. Et3N, amidation with N-Methyl-2,4-dimethylbenzylamine hydrochloride in CH2Cl2 contg. EtN(CHMe2)2 and redn. of the resulting benzamide VI with BH3 in THF.

IT 470691-98-6P 470692-06-9P 470692-08-1P
470692-09-2P 470692-10-5P 470692-11-6P
470692-12-7P 470692-13-8P

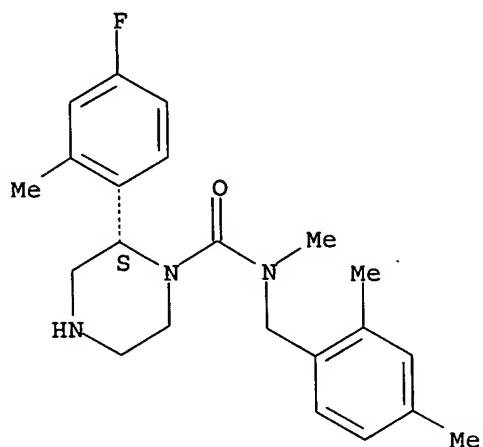
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed tachykinin antagonist; prepn. of piperazine derivs. as tachykinin antagonists)

RN 470691-98-6 CAPLUS

CN 1-Piperazinecarboxamide, N-[(2,4-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

10/089964

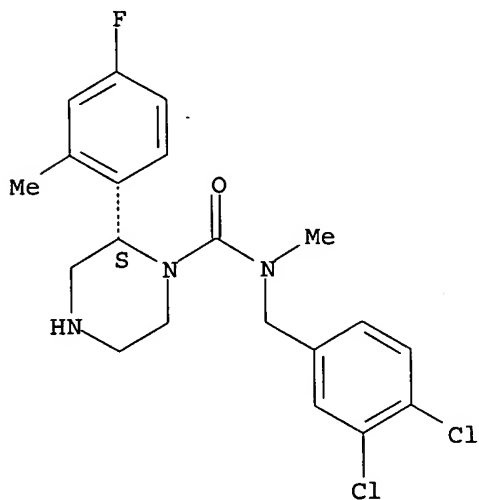
Absolute stereochemistry.



RN 470692-06-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,4-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

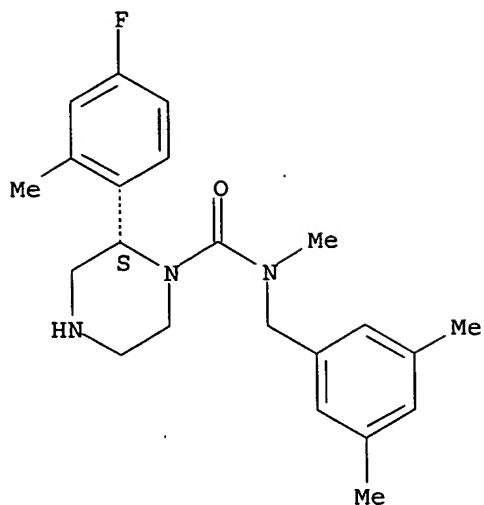


RN 470692-08-1 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

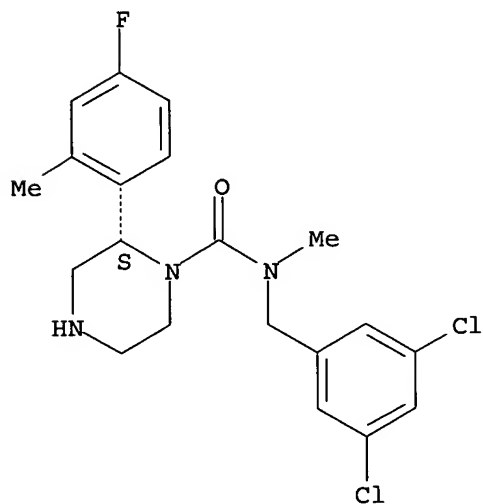
10/089964



RN 470692-09-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

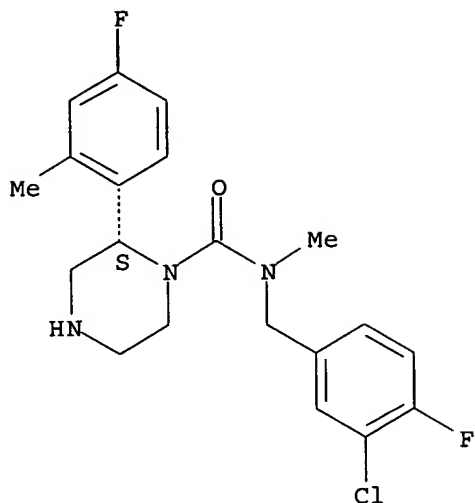


RN 470692-10-5 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3-chloro-4-fluorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

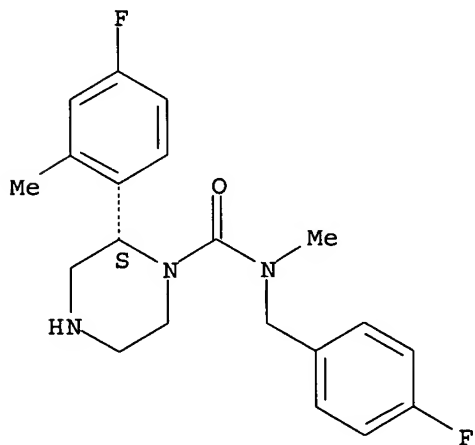
10/089964



RN 470692-11-6 CAPLUS

CN 1-Piperazinecarboxamide, 2-(4-fluoro-2-methylphenyl)-N-[(4-fluorophenyl)methyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

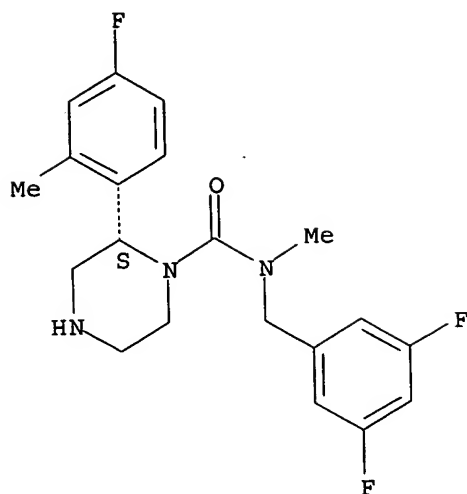


RN 470692-12-7 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-difluorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

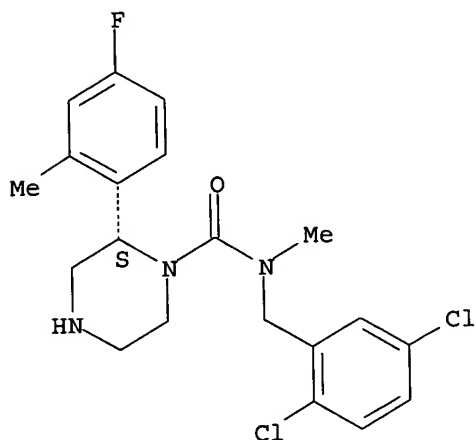
Absolute stereochemistry.

10/089964



RN 470692-13-8 CAPLUS
CN 1-Piperazinecarboxamide, N-[(2,5-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 470691-99-7P 470692-00-3P 470692-01-4P
470692-02-5P 470692-03-6P 470692-04-7P
470692-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(prepd. tachykinin antagonist; prepn. of piperazine derivs. as
tachykinin antagonists)

RN 470691-99-7 CAPLUS
CN 1-Piperazinecarboxamide, N-[(2,4-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)-, monoacetate (9CI) (CA INDEX NAME)

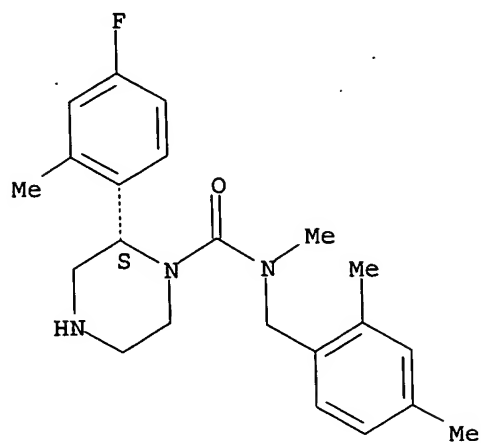
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CRN 470691-98-6

10/089964

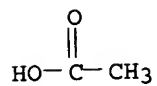
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Absolute stereochemistry.



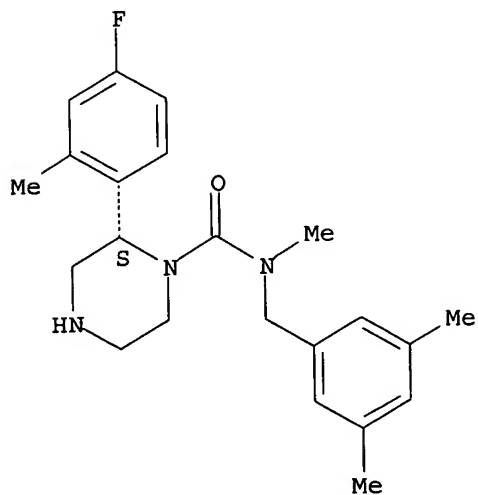
CM 2

CRN 64-19-7
CMF C2 H4 O2



RN 470692-00-3 CAPLUS
CN 1-Piperazinecarboxamide, N-[(3,5-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



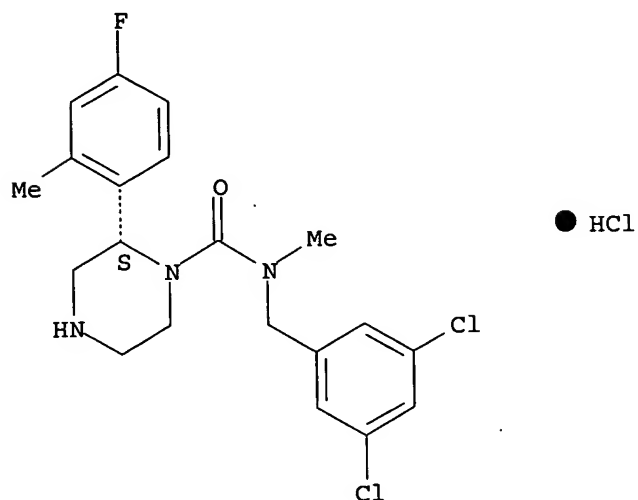
● HCl

10/089964

RN 470692-01-4 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

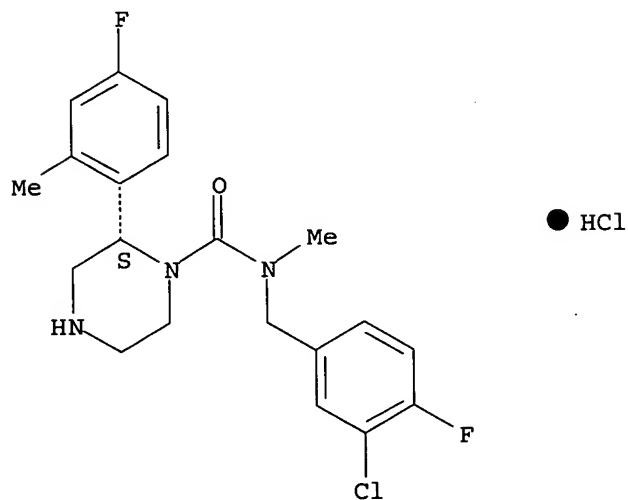
Absolute stereochemistry.



RN 470692-02-5 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3-chloro-4-fluorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

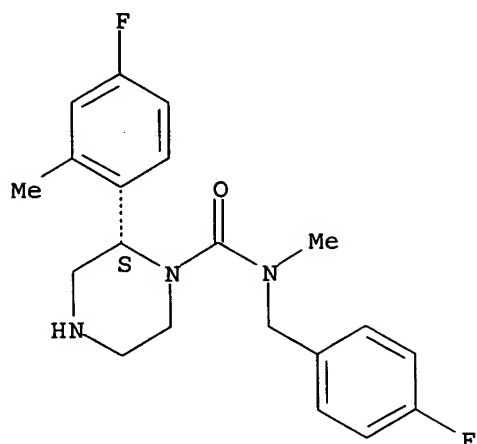


RN 470692-03-6 CAPLUS

CN 1-Piperazinecarboxamide, 2-(4-fluoro-2-methylphenyl)-N-[(4-fluorophenyl)methyl]-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

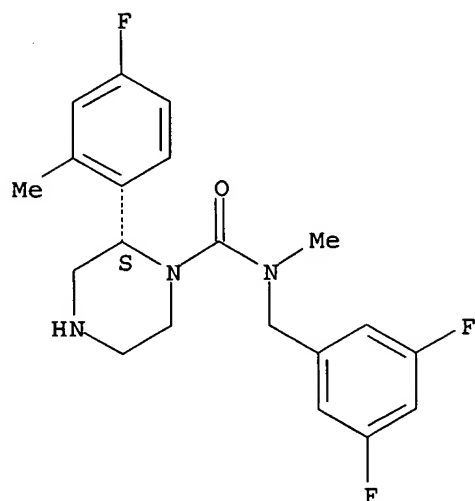
10/089964



● HCl

RN 470692-04-7 CAPLUS
CN 1-Piperazinecarboxamide, N-[(3,5-difluorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

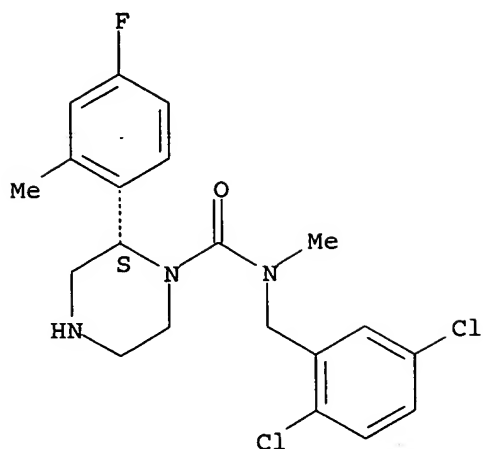


● HCl

RN 470692-05-8 CAPLUS
CN 1-Piperazinecarboxamide, N-[(2,5-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964



● HCl

IT 470692-07-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepd. tachykinin antagonist; prepn. of piperazine derivs. as tachykinin antagonists)

RN 470692-07-0 CAPLUS

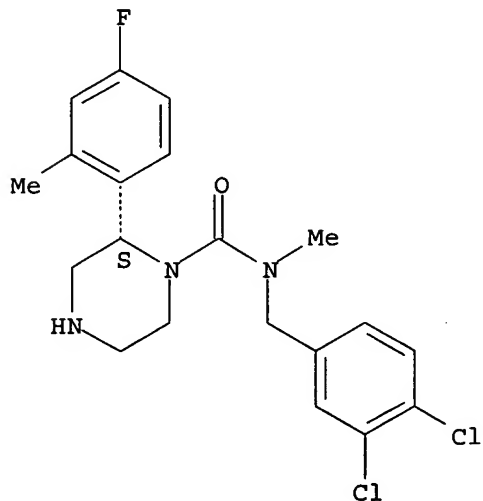
CN 1-Piperazinecarboxamide, N-[(3,4-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME).

CM 1

CRN 470692-06-9

CMF C20 H22 Cl2 F N3 O

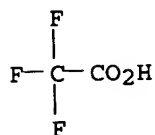
Absolute stereochemistry.



10/089964

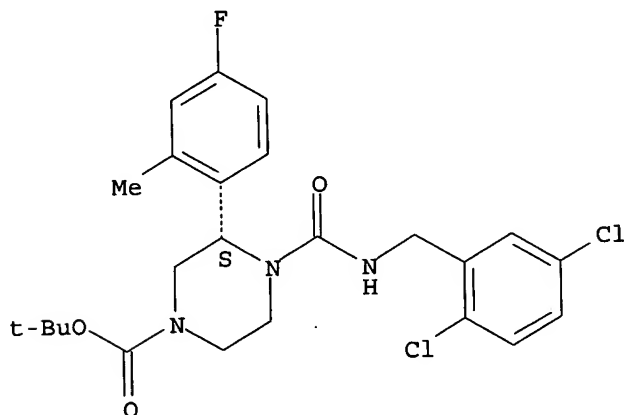
CM 2

CRN 76-05-1
CMF C2 H F3 O2



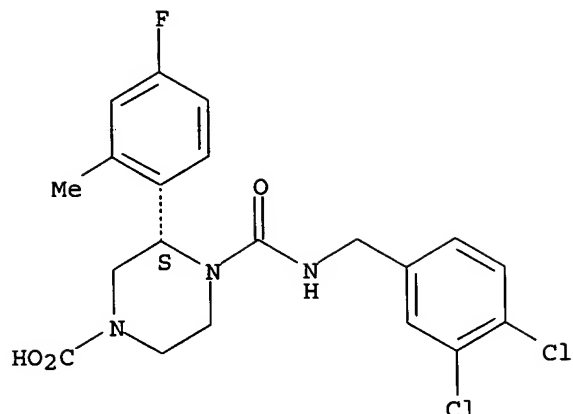
IT 470692-21-8P 470692-23-0DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and N-methylation of; prepn. of piperazine derivs. as
tachykinin antagonists)
RN 470692-21-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[(2,5-dichlorophenyl)methyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



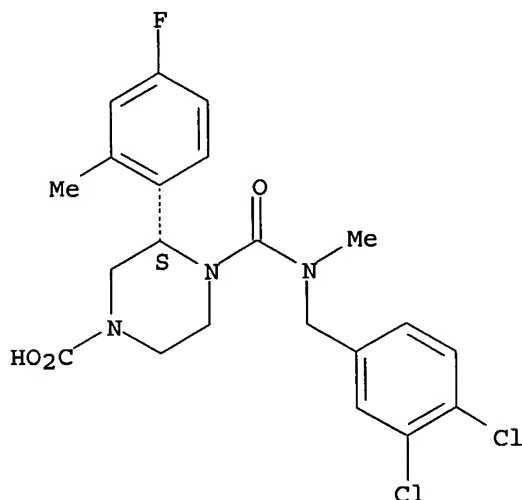
RN 470692-23-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[(3,4-dichlorophenyl)methyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 470692-24-1DP, resin-bound
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acid hydrolysis of, from resin; prepn. of piperazine derivs. as tachykinin antagonists)
 RN 470692-24-1 CAPLUS
 CN 1-Piperazinecarboxylic acid, 4-[[[(3,4-dichlorophenyl)methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (3S)- (9CI) (CA INDEX NAME)

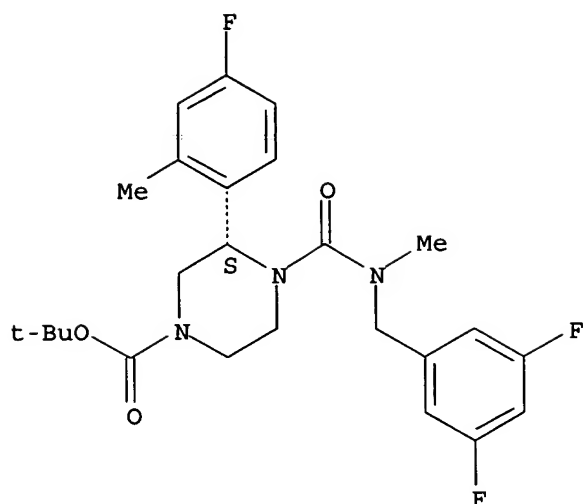
Absolute stereochemistry.



IT 470692-20-7P 470692-22-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and acid hydrolysis of; prepn. of piperazine derivs. as tachykinin antagonists)
 RN 470692-20-7 CAPLUS
 CN 1-Piperazinecarboxylic acid, 4-[[[(3,5-difluorophenyl)methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

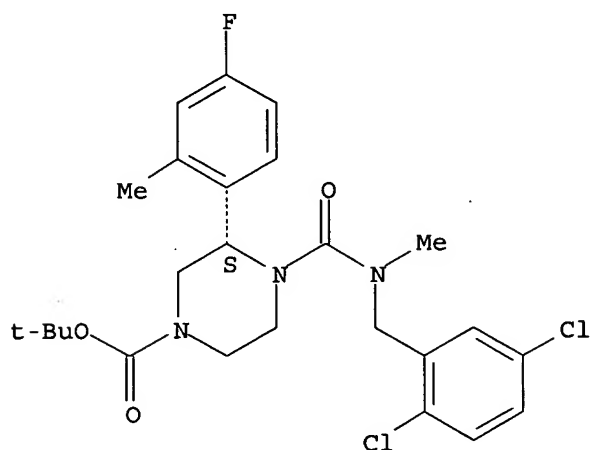
10/089964



RN 470692-22-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(2,5-dichlorophenyl)methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 470692-14-9P 470692-15-0P 470692-16-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

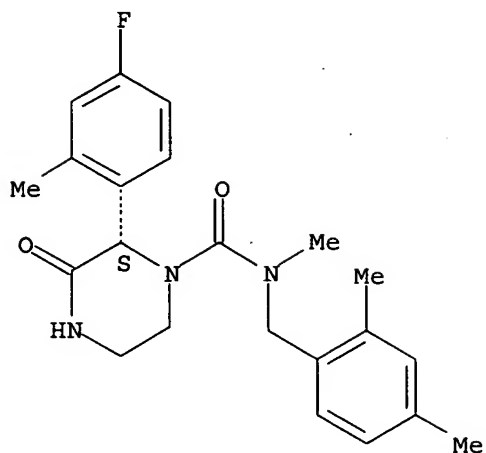
(prepn. and borane redn. of; prepn. of piperazine derivs. as tachykinin antagonists)

RN 470692-14-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[(2,4-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo-, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

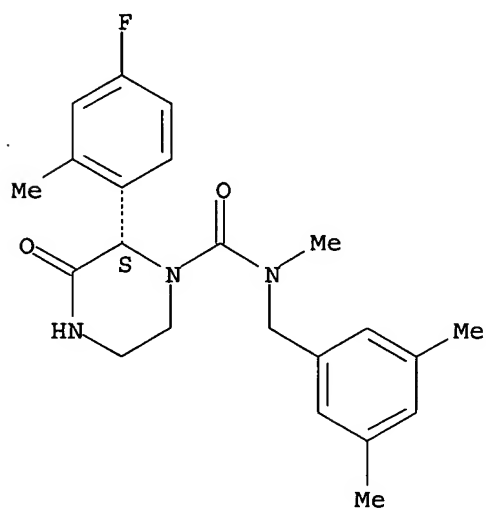
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RN 470692-15-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-dimethylphenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo-, (2S)- (9CI) (CA INDEX NAME)

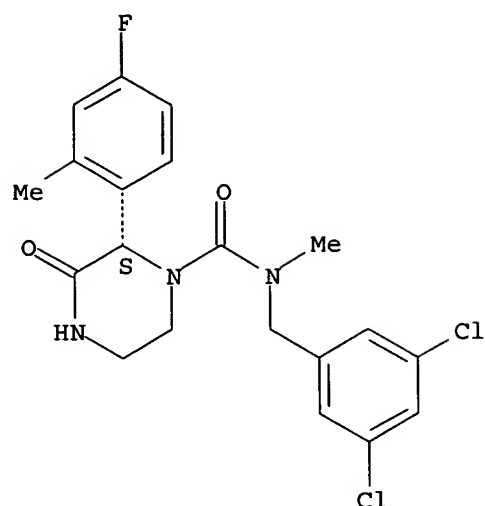
Absolute stereochemistry.



RN 470692-16-1 CAPLUS

CN 1-Piperazinecarboxamide, N-[(3,5-dichlorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 470692-17-2P 470692-18-3P

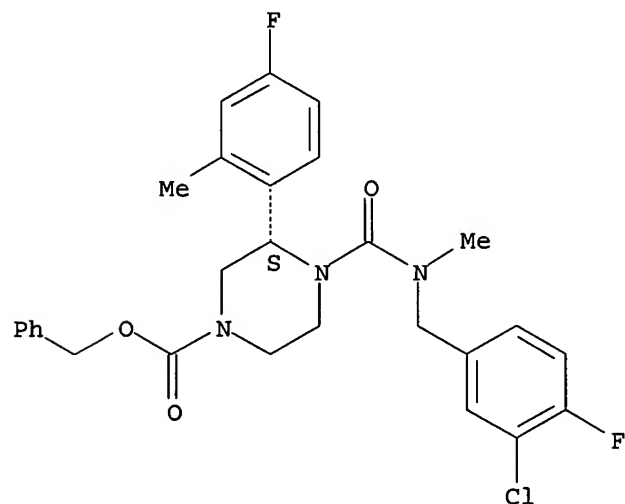
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and palladium-catalyzed hydrogenolysis of; prepn. of piperazine derivs. as tachykinin antagonists)

RN 470692-17-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(3-chloro-4-fluorophenyl)methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

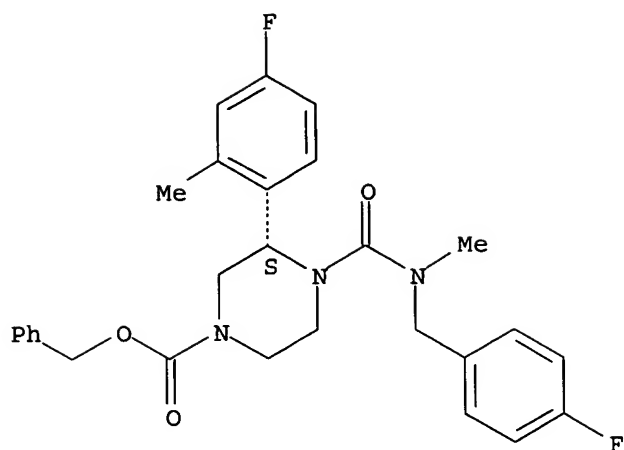


RN 470692-18-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 3-(4-fluoro-2-methylphenyl)-4-[[[(4-fluorophenyl)methyl]methylamino]carbonyl]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS
 AN 2001:265403 CAPLUS
 DN 134:295839
 TI Preparation of 2-phenylpiperazine-1-carboxylic acid benzylamides as
 tachykinin antagonists
 IN Alvaro, Giuseppe; Di Fabio, Romano; Giovannini, Riccardo; Guercio,
 Giuseppe; St. Denis, Yves; Ursini, Antonella
 PA Glaxo Group Limited, UK
 SO PCT Int. Appl., 103 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001025219	A2	20010412	WO 2000-EP9722	20001005
	WO 2001025219	A3	20011213		
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	US 2003028021	A1	20030206	US 2002-190170	20020703
PRAI	GB 1999-23748	A	19991007		
	WO 2000-EP9722	W	20001005		
	US 2002-89964	A1	20020508		
OS	MARPAT 134:295839				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to piperazine derivs. I [wherein: R = halo, C1-4 alkyl; R1 = H, C1-4 alkyl; R2 = H, C1-4 alkyl, C2-6 alkenyl, C3-7 cycloalkyl; or NR1CR2 = 5- to 6-membered heterocyclyl; R3 = CF3, C1-4 alkyl, C1-4 alkoxy, CF3O, or halo; R4 = H, (CH2)qR7 or (CH2)rCO(CH2)pR7; R5 = H, C1-4 alkyl or COR6; R6 = H, OH, NH2, NHMe, NMe2, 5-membered heteroaryl contg. 1-3 N/O/S or 6-membered heteroaryl contg. 1-3 N atoms; R7 = H, OH, or NR8R9 wherein R8 and R9 = H or C1-4 alkyl (un)substituted by OH or by NH2; R10 = H, C1-4 alkyl; or R10 and R2 form C3-7 cycloalkyl; m, n = 0-3; p, r = 0-4; q = 1-4; provided that, when NR1CR2 = 5- to 6-membered heterocyclic, then (i) m = 1 or 2; (ii) when m = 1, R .noteq. F; and (iii) when m = 2, both R .noteq. F] and pharmaceutically acceptable salts and solvates thereof. The compds. are potent and specific antagonists of tachykinins, including substance P and other neurokinins. Examples include 38 syntheses, 82 preps. of intermediates, 4 std. formulations, and 2 bioassays. For instance, (+)-(S)-3-(4-fluoro-2-methylphenyl)piperazin-2-one (prepn. given) was treated with triphosgene

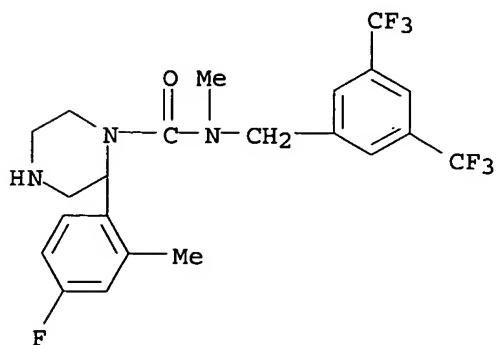
and amidated with 3,5-(F3C)2C6H3CHMeNHMe to give 2 diastereomeric amides. Sepn. of the (S,S)-diastereomer by flash chromatog. and redn. of the ring oxo group with BH3.THF gave title compd. II, isolated as the acetate salt (III). Using the gerbil foot-tapping model for reversal of an NK1 agonist, III had an oral ED50 of 0.04 mg/kg.

IT 334476-29-8P 334476-30-1P 334476-31-2P
 334476-32-3P 334476-33-4P 334476-34-5P
 334476-35-6P 334476-36-7P 334476-37-8P
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 334476-44-7P 334476-45-8P 334476-46-9P
 334476-47-0P 334476-48-1P 334476-49-2P
 334476-50-5P 334476-51-6P 334476-52-7P
 334476-53-8P 334476-54-9P 334476-55-0P
 334476-56-1P 334476-57-2P 334476-58-3P
 334476-59-4P 334476-60-7P 334476-61-8P
 334476-62-9P 334476-63-0P 334476-64-1P
 334476-65-2P 334476-66-3P 334476-67-4P
 334476-68-5P 334476-69-6P 334476-70-9P
 334476-71-0P 334476-72-1P 334476-73-2P
 334476-74-3P 334476-75-4P 334476-76-5P
 334476-77-6P 334476-78-7P 334476-79-8P
 334476-80-1P 334476-81-2P 334476-82-3P
 334476-83-4P 334476-84-5P 334476-85-6P
 334476-86-7P 334823-44-8P 334823-46-0P
 334825-32-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; prepn. of phenylpiperazinecarboxylic acid benzylamides as tachykinin antagonists)

RN 334476-29-8 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

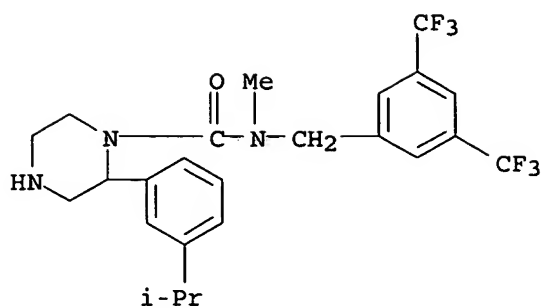


● HCl

RN 334476-30-1 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

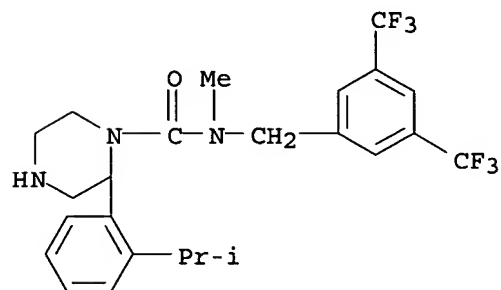
10/089964



● HCl

RN 334476-31-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-[2-(1-methylethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

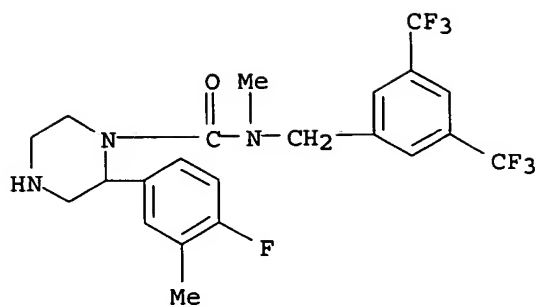


● HCl

RN 334476-32-3 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-3-methylphenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

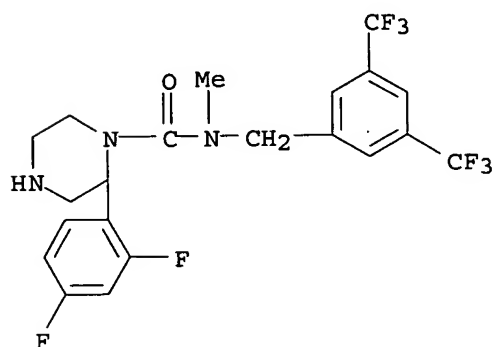
10/089964



● HCl

RN 334476-33-4 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(2,4-difluorophenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

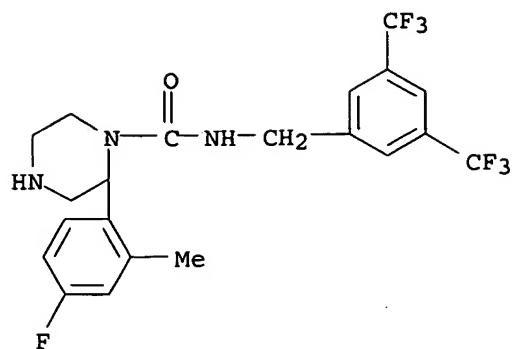


● HCl

RN 334476-34-5 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

10/089964

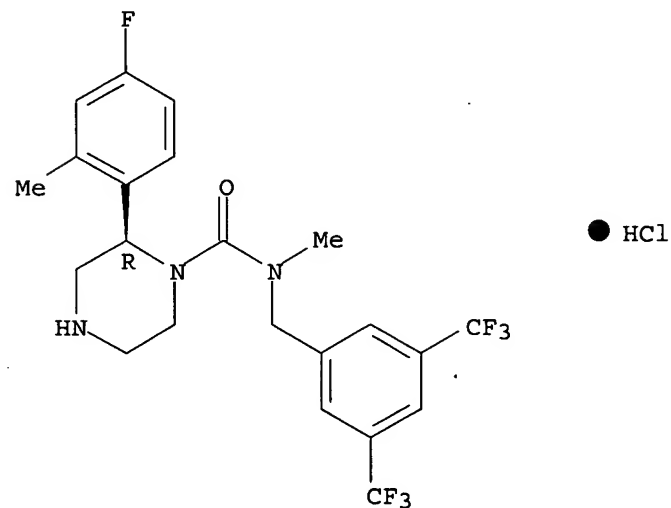


● HCl

RN 334476-35-6 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



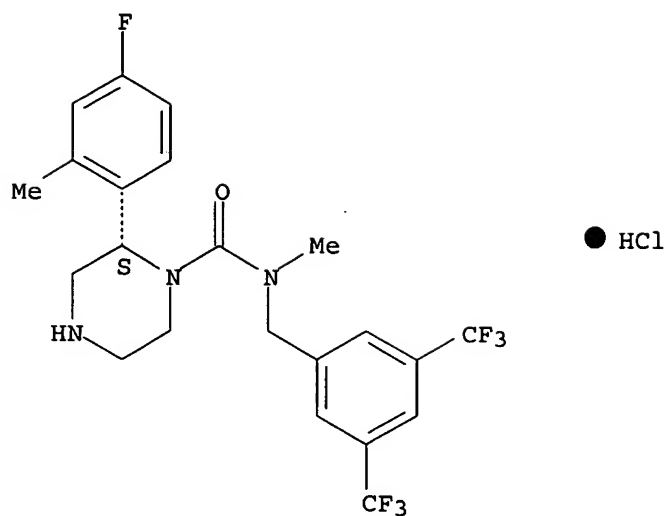
● HCl

RN 334476-36-7 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

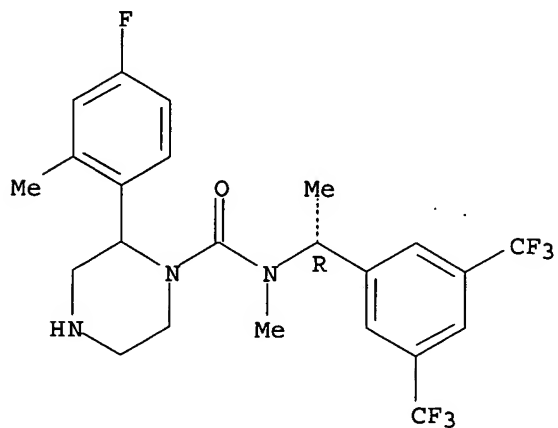
Absolute stereochemistry. Rotation (-).

10/089964



RN 334476-37-8 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

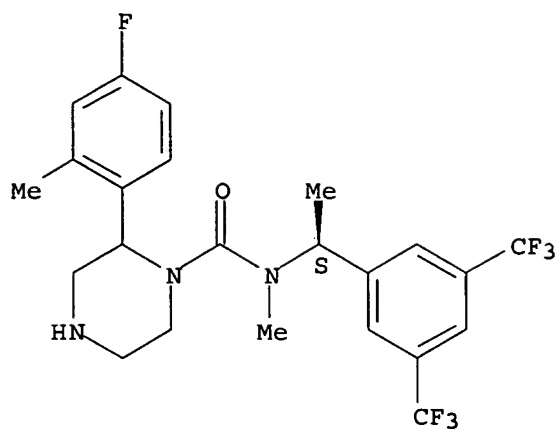
Absolute stereochemistry.



RN 334476-38-9 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

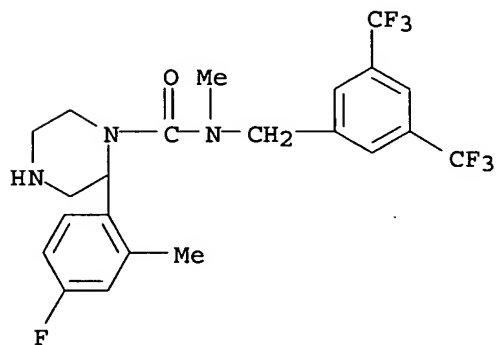
10/089964



● HCl

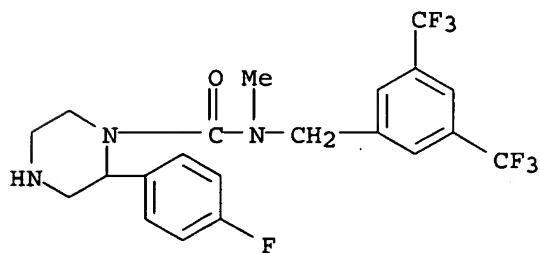
RN 334476-39-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-40-3 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluorophenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

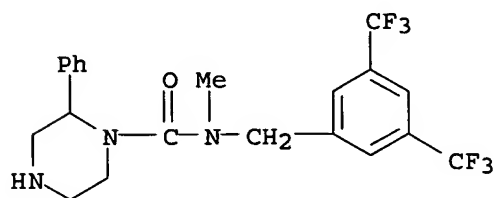


HCl

10/089964

RN 334476-41-4 CAPLUS

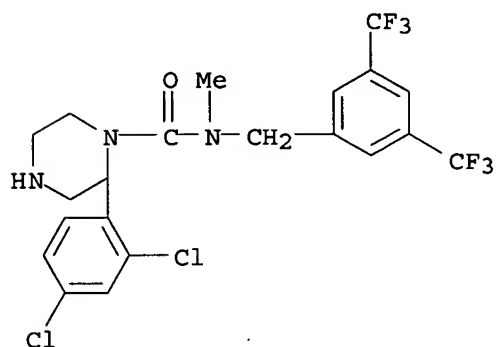
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 334476-42-5 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(2,4-dichlorophenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

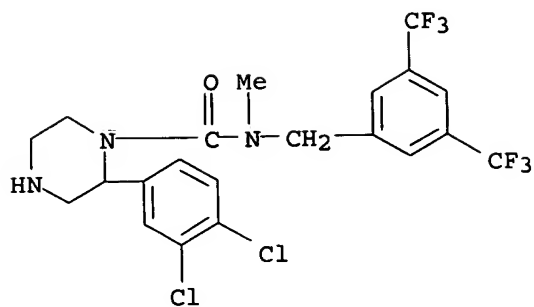


● HCl

RN 334476-43-6 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(3,4-dichlorophenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

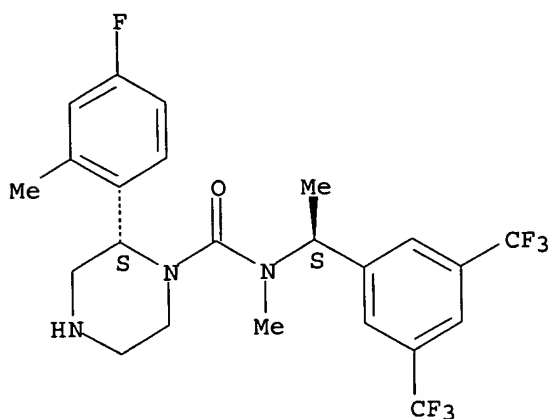
10/089964



● HCl

RN 334476-44-7 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-
2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (-).

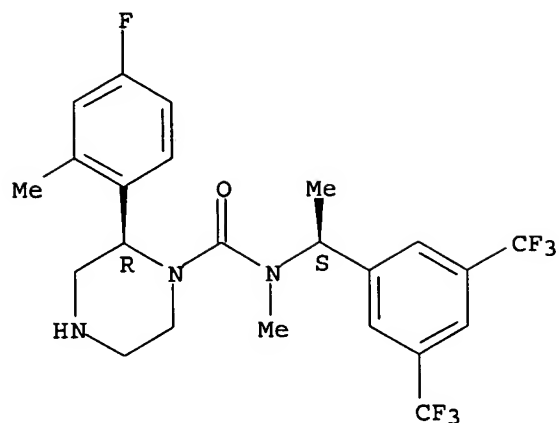


● HCl

RN 334476-45-8 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-
2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2R)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (+).

10/089964

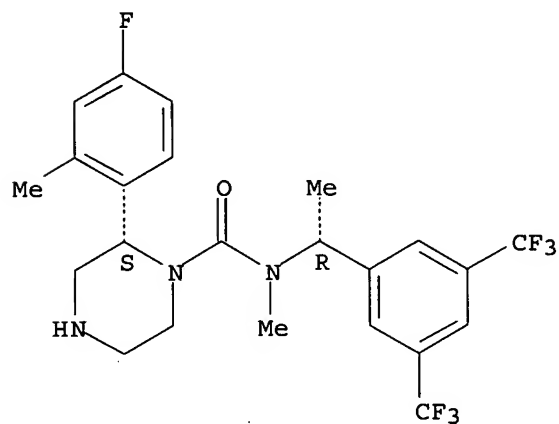


● HCl

RN 334476-46-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-
2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 334476-47-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-
2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)-, monoacetate (9CI) (CA INDEX
NAME)

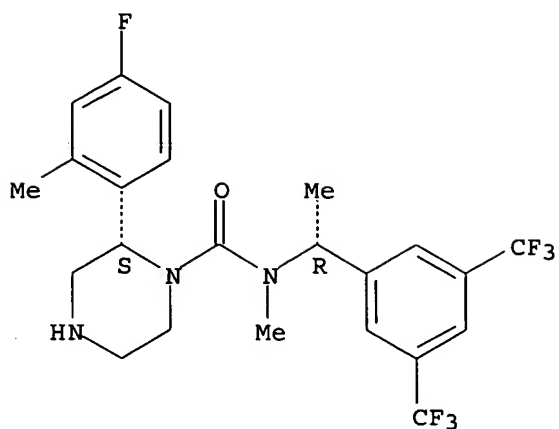
CM 1

CRN 334476-46-9

CMF C23 H24 F7 N3 O

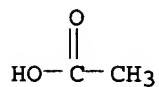
Absolute stereochemistry. Rotation (+).

10/089964



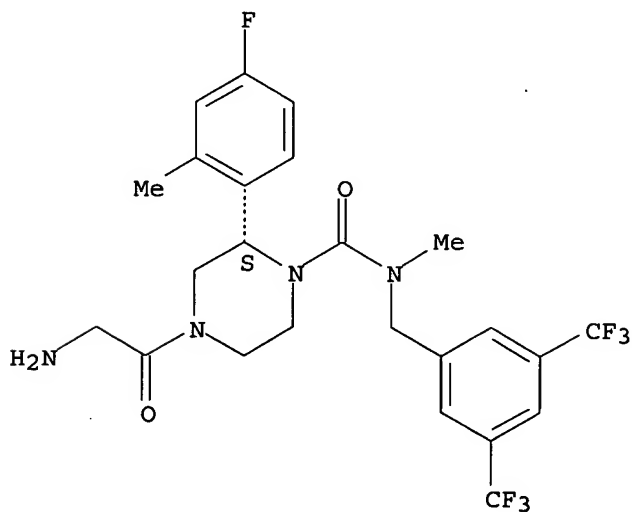
CM 2

CRN 64-19-7
CMF C2 H4 O2



RN 334476-48-1 CAPLUS
CN 1-Piperazinecarboxamide, 4-(aminoacetyl)-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



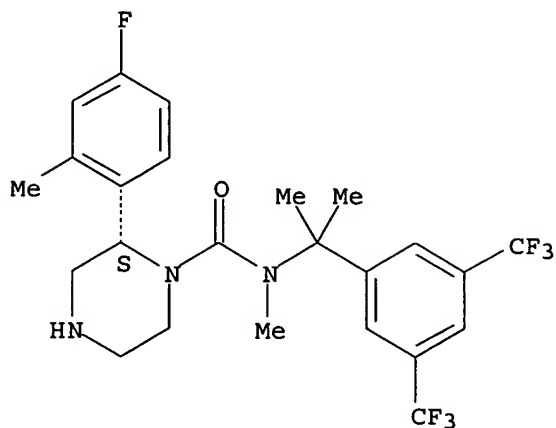
● HCl

RN 334476-49-2 CAPLUS
CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]-1-methylethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride,

10/089964

(2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

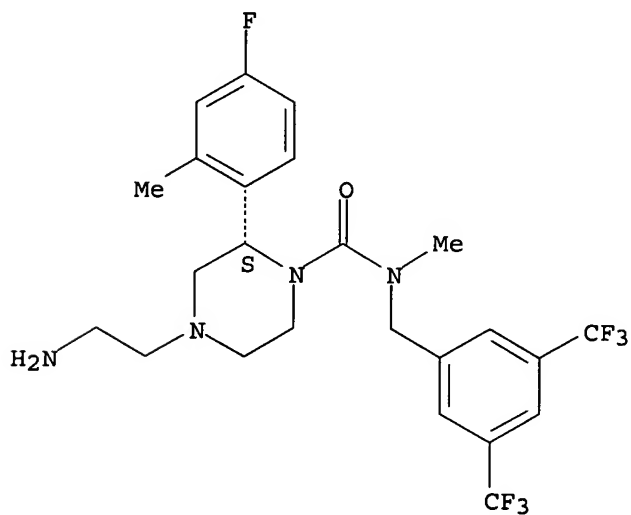


● HCl

RN 334476-50-5 CAPLUS

CN 1-Piperazinecarboxamide, 4-(2-aminoethyl)-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

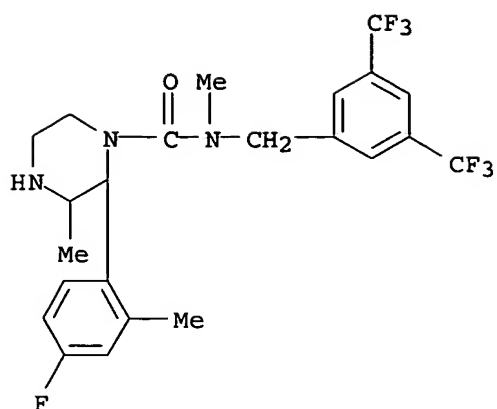


●2 HCl

RN 334476-51-6 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N,3-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

10/089964

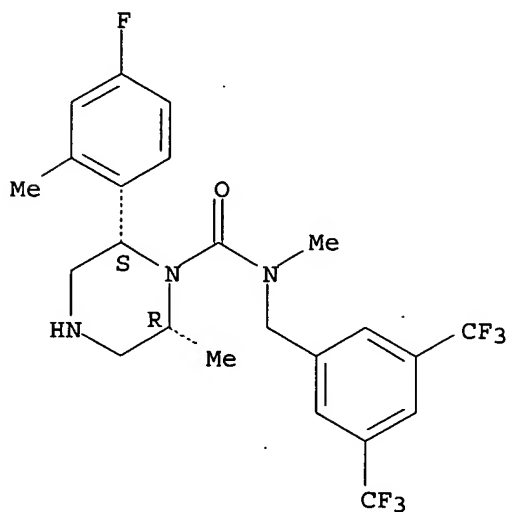


● HCl

RN 334476-52-7 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N,6-dimethyl-, monohydrochloride, (2R,6S)-rel-
(9CI) (CA INDEX NAME)

Relative stereochemistry.

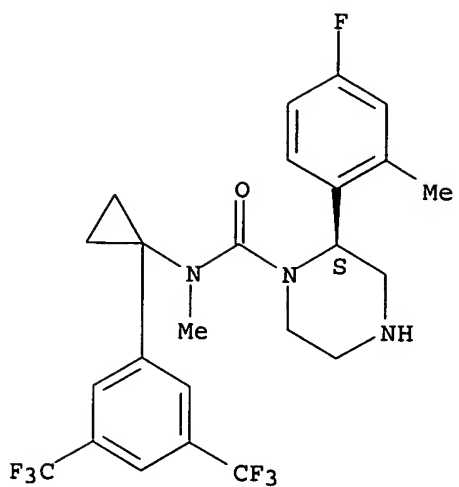


● HCl

RN 334476-53-8 CAPLUS

CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]cyclopropyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

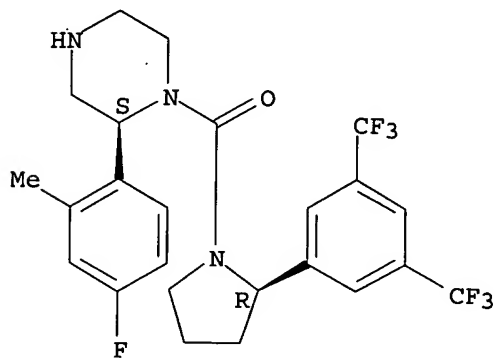
Absolute stereochemistry.



● HCl

RN 334476-54-9 CAPLUS
 CN Piperazine, 1-[[(2R)-2-[3,5-bis(trifluoromethyl)phenyl]-1-pyrrolidinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

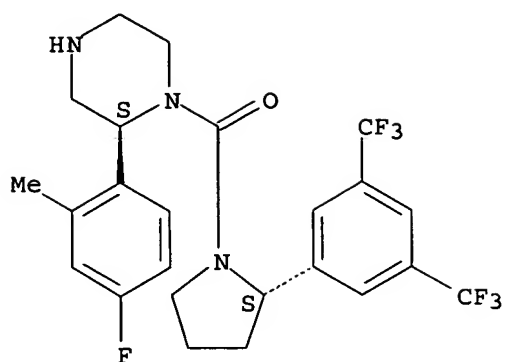


● HCl

RN 334476-55-0 CAPLUS
 CN Piperazine, 1-[[(2S)-2-[3,5-bis(trifluoromethyl)phenyl]-1-pyrrolidinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964



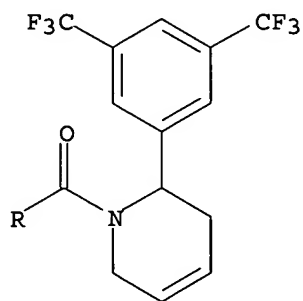
● HCl

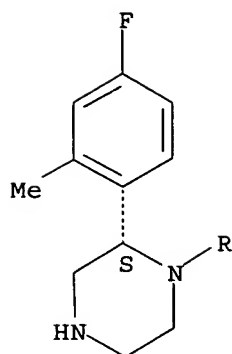
RN 334476-56-1 CAPLUS

CN Piperazine, 1-[[2-[3,5-bis(trifluoromethyl)phenyl]-3,6-dihydro-1(2H)-pyridinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, monohydrochloride, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

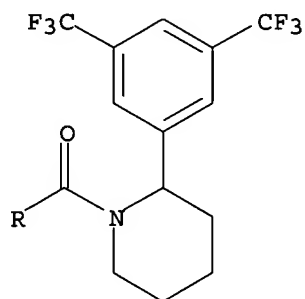


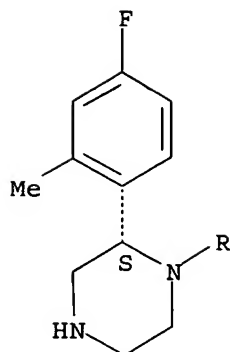


● HCl

RN 334476-57-2 CAPLUS
 CN Piperazine, 1-[[2-[3,5-bis(trifluoromethyl)phenyl]-1-piperidinyl]carbonyl]-
 2-(4-fluoro-2-methylphenyl)-, monohydrochloride, (2S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



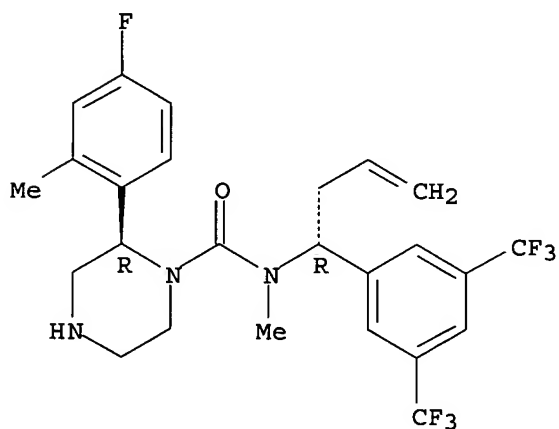


● HCl

RN 334476-58-3 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



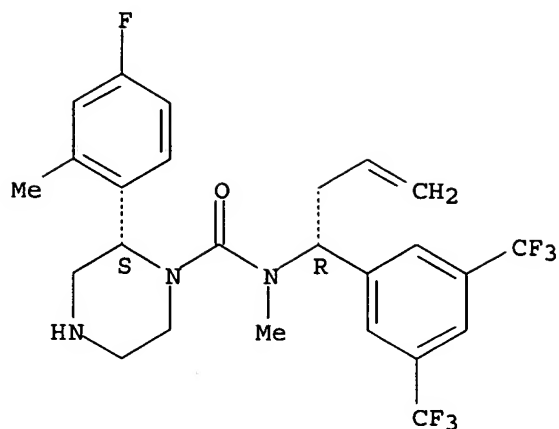
● HCl

RN 334476-59-4 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

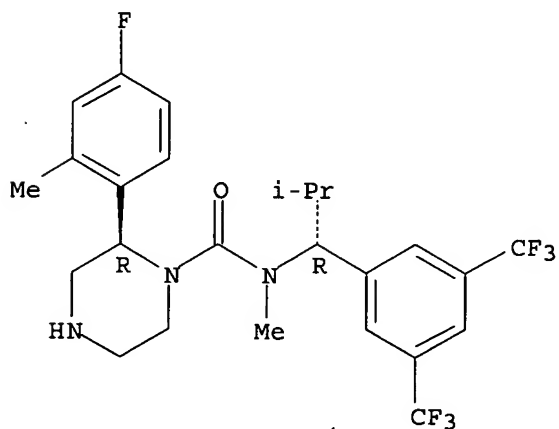
10/089964



● HCl

RN 334476-60-7 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

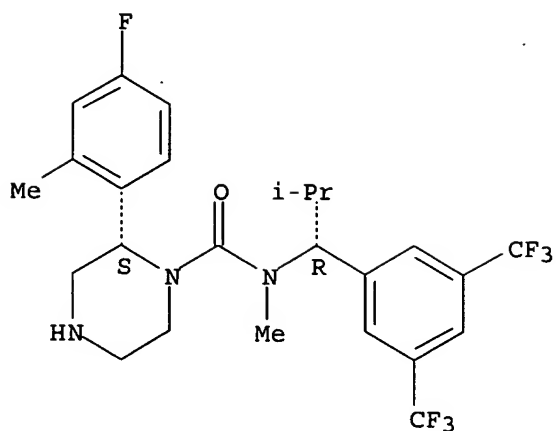


● HCl

RN 334476-61-8 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)-rel- (9CI) (CA INDEX NAME)

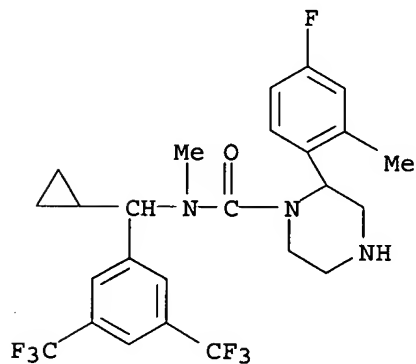
Relative stereochemistry.

10/089964



● HCl

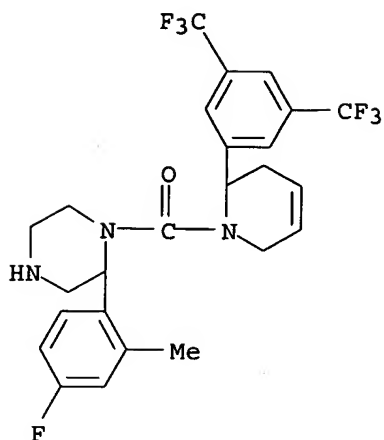
RN 334476-62-9 CAPLUS
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]cyclopropylmethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 334476-63-0 CAPLUS
CN Piperazine, 1-[[2-[[3,5-bis(trifluoromethyl)phenyl]-3,6-dihydro-1(2H)-pyridinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

10/089964



● HCl

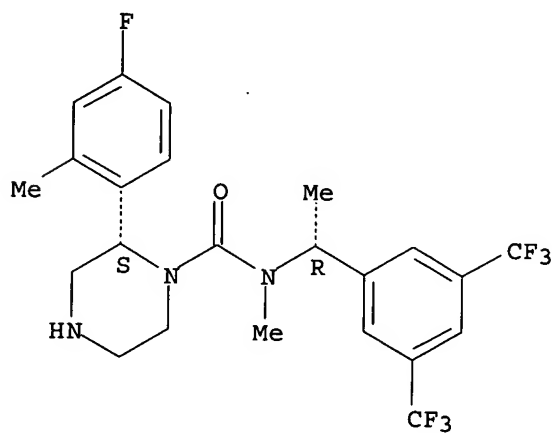
RN 334476-64-1 CAPLUS
CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-
2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)-, monomethanesulfonate (9CI)
(CA INDEX NAME)

CM 1

CRN 334476-46-9

CMF C23 H24 F7 N3 O

Absolute stereochemistry. Rotation (+).

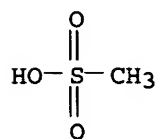


CM 2

CRN 75-75-2

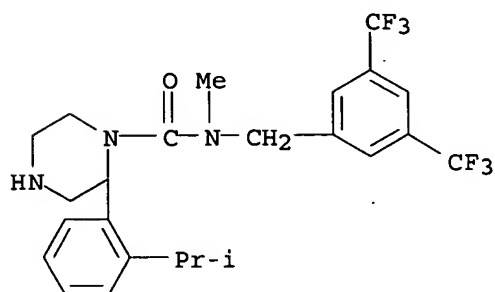
CMF C H4 O3 S

10/089964



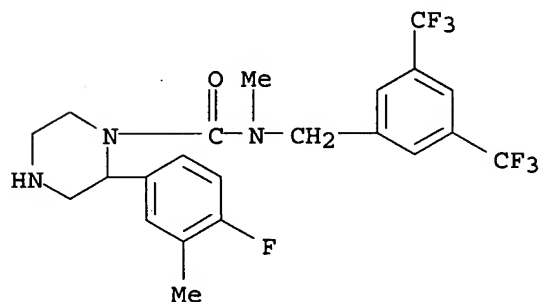
RN 334476-65-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-[2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 334476-66-3 CAPLUS

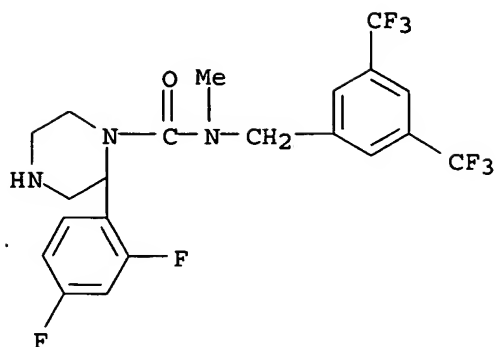
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-3-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-67-4 CAPLUS

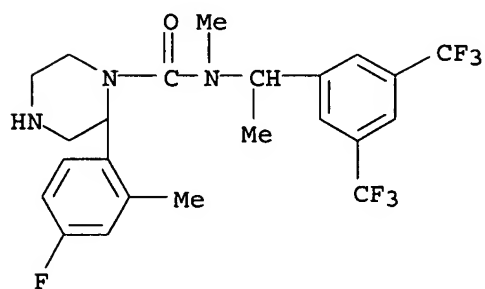
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(2,4-difluorophenyl)-N-methyl- (9CI) (CA INDEX NAME)

10/089964



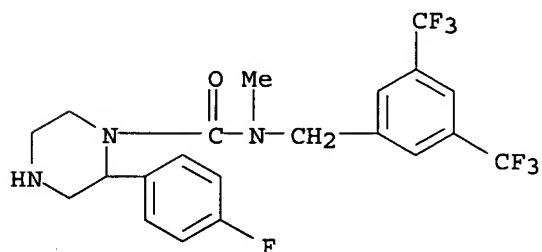
RN 334476-68-5 CAPLUS

CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-69-6 CAPLUS

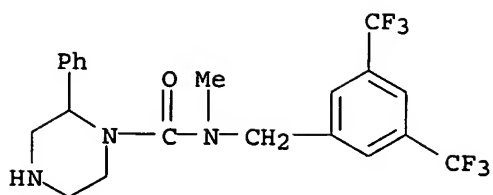
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluorophenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-70-9 CAPLUS

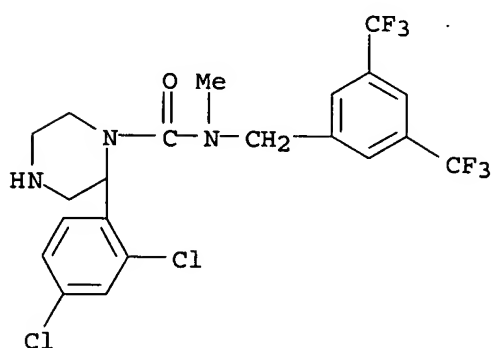
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-phenyl- (9CI) (CA INDEX NAME)

10/089964



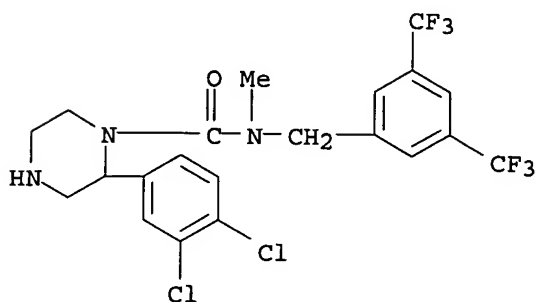
RN 334476-71-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(2,4-dichlorophenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-72-1 CAPLUS

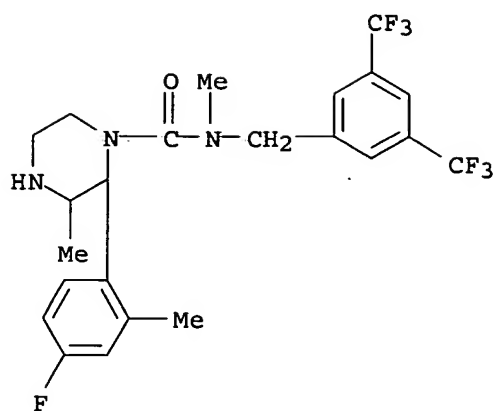
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(3,4-dichlorophenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-73-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N,3-dimethyl- (9CI) (CA INDEX NAME)

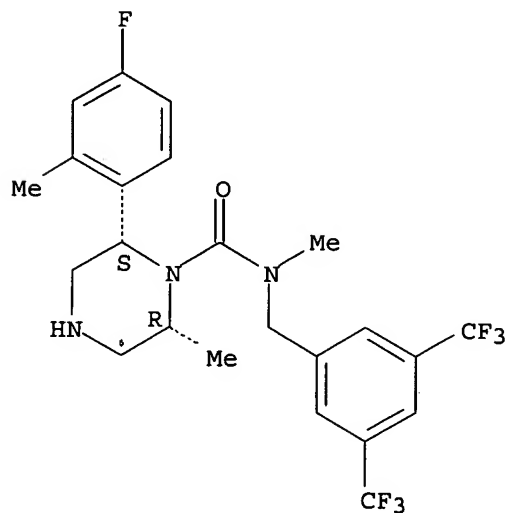
10/089964



RN 334476-74-3 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N,6-dimethyl-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

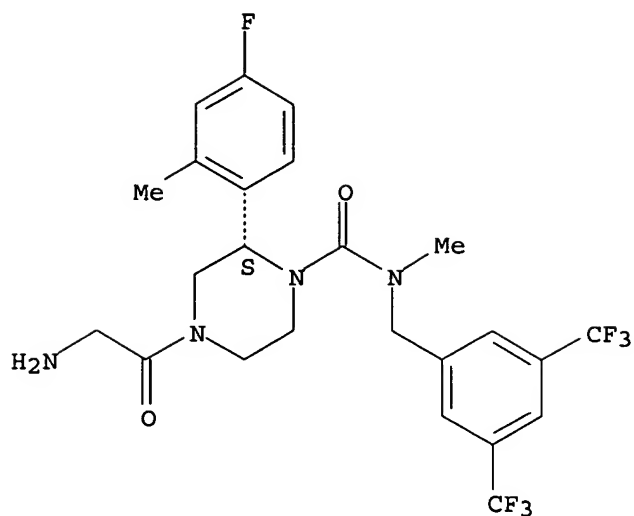


RN 334476-75-4 CAPLUS

CN 1-Piperazinecarboxamide, 4-(aminoacetyl)-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

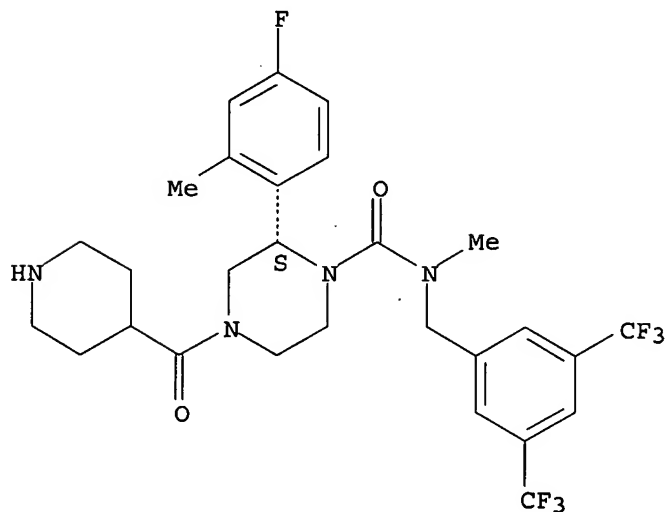
Absolute stereochemistry.

10/089964



RN 334476-76-5 CAPLUS
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-4-(4-piperidinylcarbonyl)-, (2S)- (9CI)
(CA INDEX NAME)

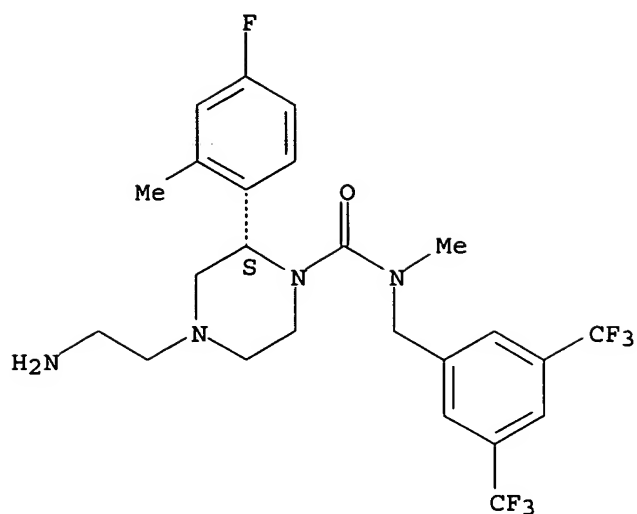
Absolute stereochemistry.



RN 334476-77-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(2-aminoethyl)-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

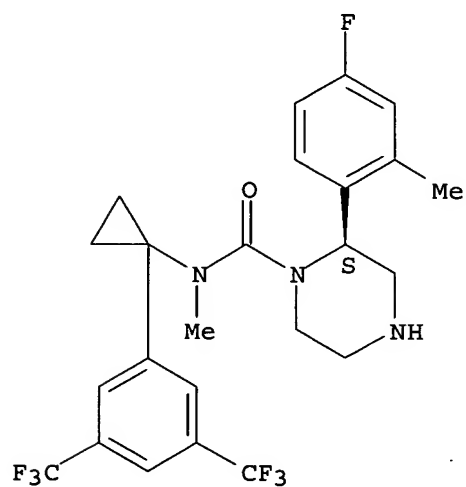
10/089964



RN 334476-78-7 CAPLUS

CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]cyclopropyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

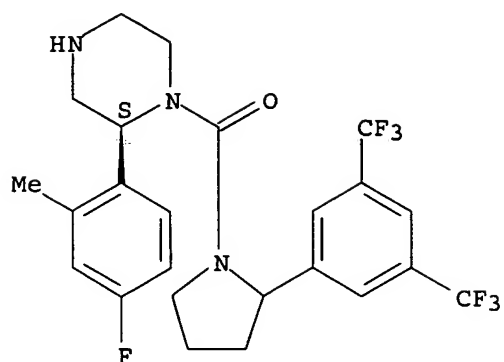


RN 334476-79-8 CAPLUS

CN Piperazine, 1-[[2-[3,5-bis(trifluoromethyl)phenyl]-1-cyclopropyl]-1-pyrrolidinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964

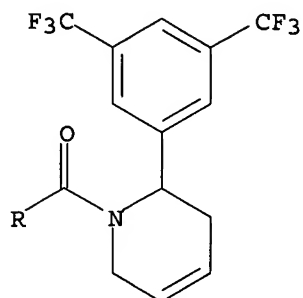


RN 334476-80-1 CAPLUS

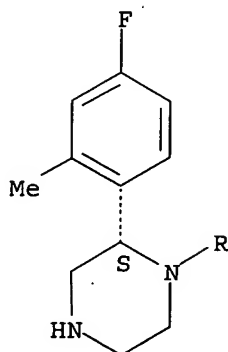
CN Piperazine, 1-[[2-[3,5-bis(trifluoromethyl)phenyl]-3,6-dihydro-1(2H)-pyridinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



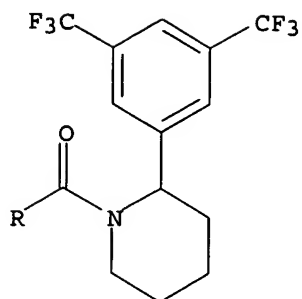
RN 334476-81-2 CAPLUS

CN Piperazine, 1-[[2-[3,5-bis(trifluoromethyl)phenyl]-1-piperidinyl]carbonyl]-2-(4-fluoro-2-methylphenyl)-, (2S)- (9CI) (CA INDEX NAME)

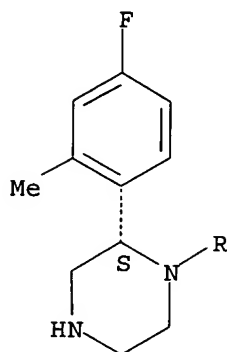
10/089964

Absolute stereochemistry.

PAGE 1-A

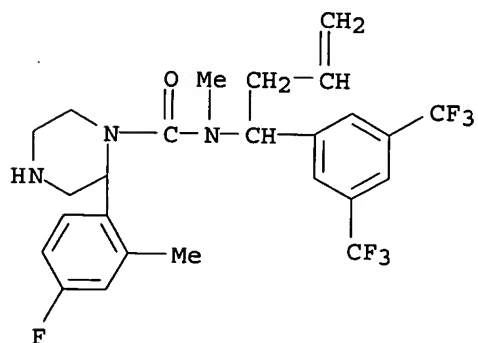


PAGE 2-A



RN 334476-82-3 CAPLUS

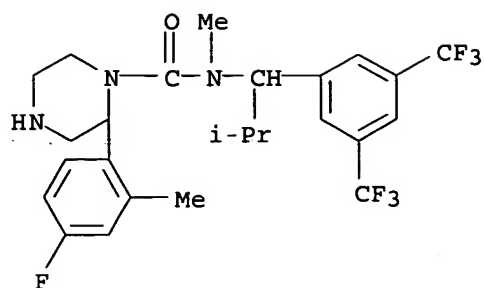
CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-83-4 CAPLUS

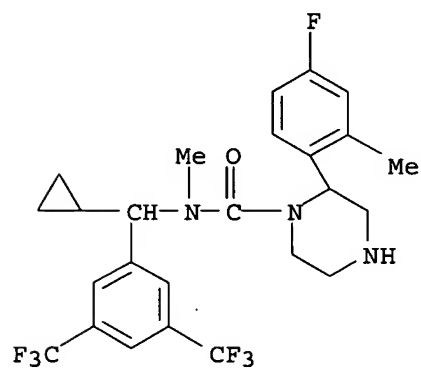
CN 1-Piperazinecarboxamide, N-[1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)

10/089964



RN 334476-84-5 CAPLUS

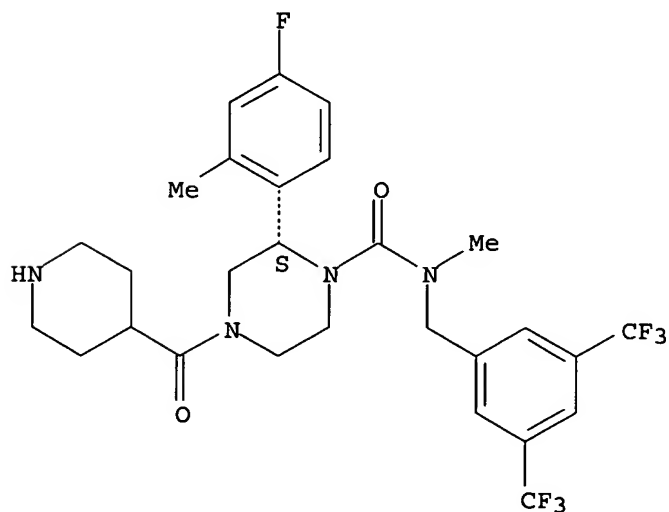
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]cyclopropylmethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334476-85-6 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-4-(4-piperidinylcarbonyl)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

10/089964

RN 334476-86-7 CAPLUS

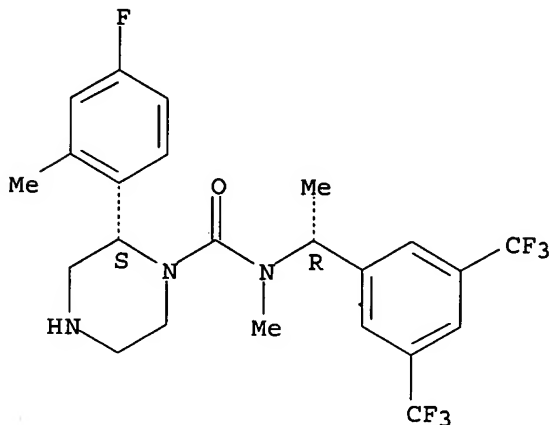
CN Ethanesulfonic acid, compd. with (2S)-N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-1-piperazinecarboxamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 334476-46-9

CMF C23 H24 F7 N3 O

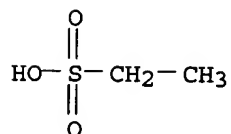
Absolute stereochemistry. Rotation (+).



CM 2

CRN 594-45-6

CMF C2 H6 O3 S

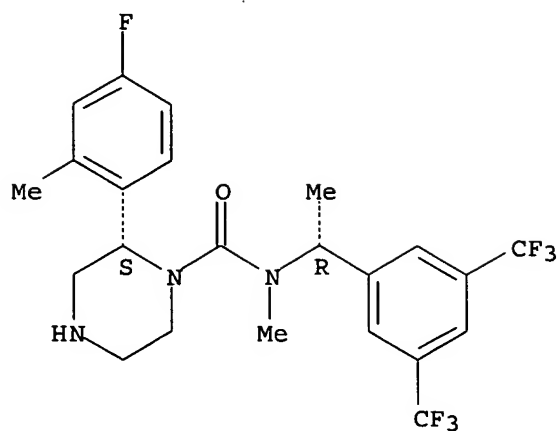


RN 334823-44-8 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

10/089964

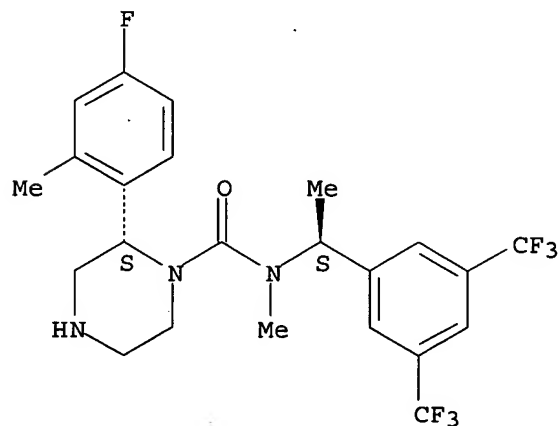


● HCl

RN 334823-46-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 334825-32-0 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)-, monoacetate (9CI) (CA INDEX NAME)

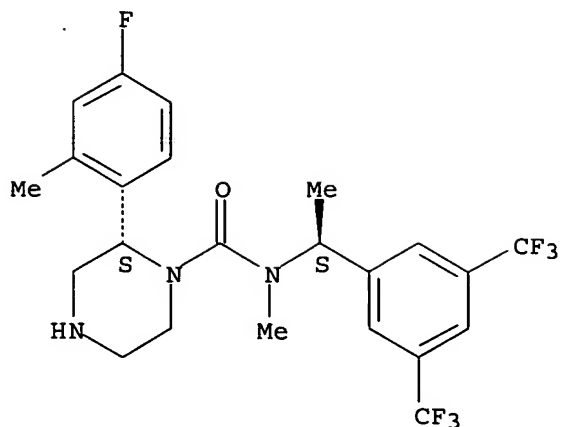
CM 1

CRN 334823-46-0

CMF C23 H24 F7 N3 O

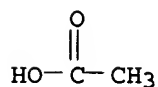
Absolute stereochemistry. Rotation (-).

10/089964



CM 2

CRN 64-19-7
CMF C2 H4 O2



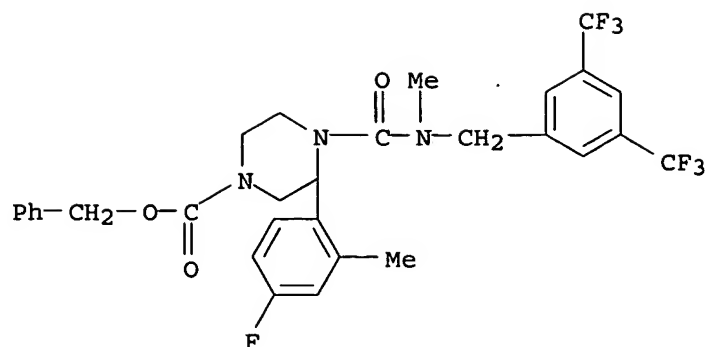
IT 334476-98-1P 334476-99-2P 334477-00-8P
334477-01-9P 334477-02-0P 334477-03-1P
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334477-12-2P 334477-13-3P 334477-14-4P
334477-15-5P 334477-16-6P 334477-17-7P
334477-19-9P 334477-20-2P 334477-24-6P
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334477-73-5P 334477-77-9P 334477-78-0P
334477-79-1P 334477-80-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; prepn. of phenylpiperazinecarboxylic acid benzylamides
as tachykinin antagonists)

RN 334476-98-1 CAPLUS

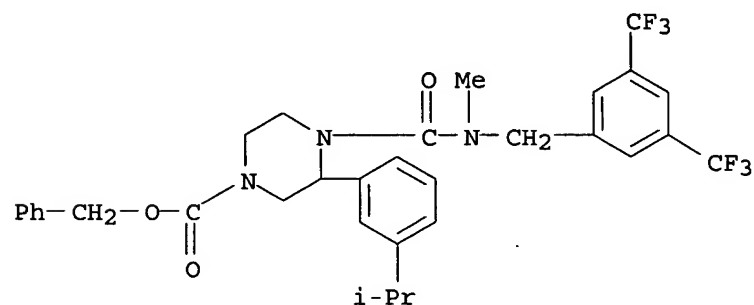
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]m
ethylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester
(9CI) (CA INDEX NAME)

10/089964



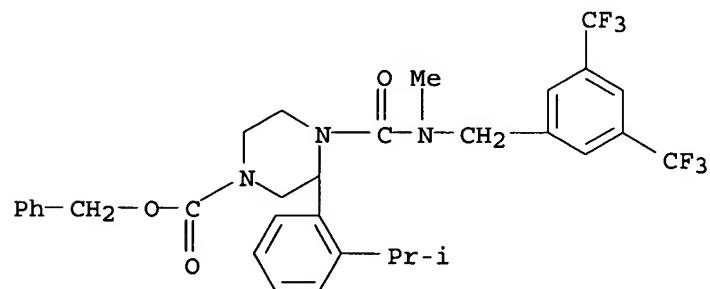
RN 334476-99-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylethylamino]carbonyl]-3-[3-(1-methylethyl)phenyl]-, phenylmethyl ester
(9CI) (CA INDEX NAME)



RN 334477-00-8 CAPLUS

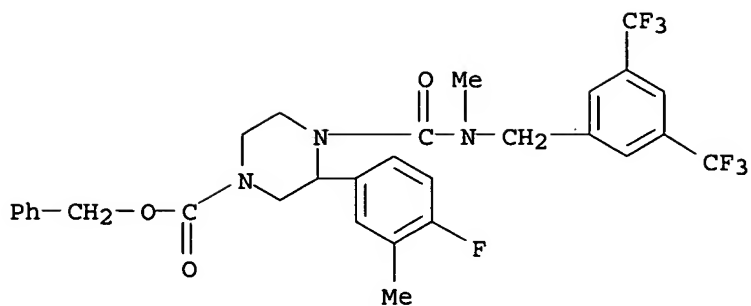
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylethylamino]carbonyl]-3-[2-(1-methylethyl)phenyl]-, phenylmethyl ester
(9CI) (CA INDEX NAME)



RN 334477-01-9 CAPLUS

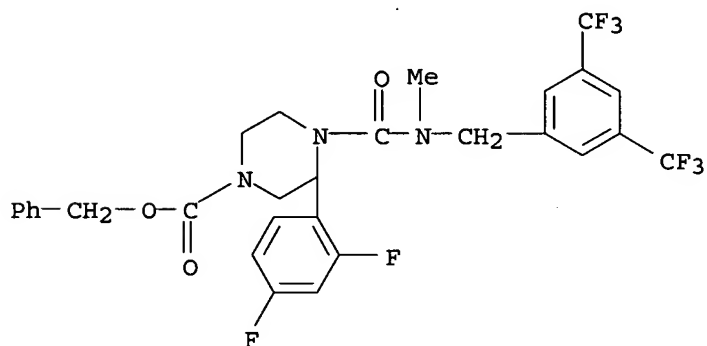
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylethylamino]carbonyl]-3-(4-fluoro-3-methylphenyl)-, phenylmethyl ester
(9CI) (CA INDEX NAME)

10/089964



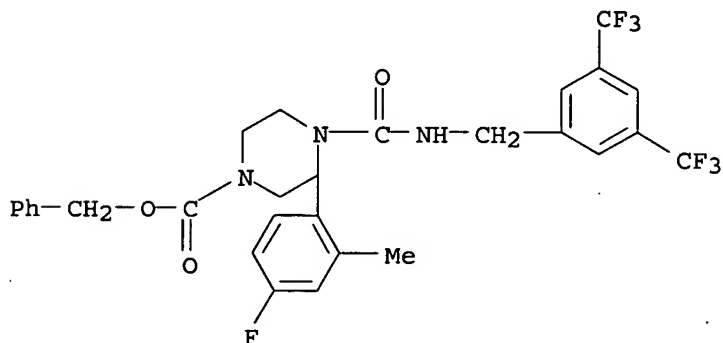
RN 334477-02-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylamino]carbonyl]-3-(2,4-difluorophenyl)-, phenylmethyl ester (9CI)
(CA INDEX NAME)



RN 334477-03-1 CAPLUS

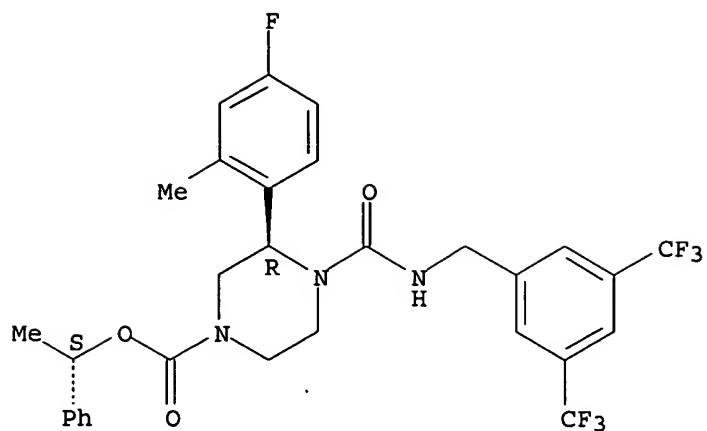
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 334477-05-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1S)-1-phenylethyl ester, (3R)- (9CI) (CA INDEX NAME)

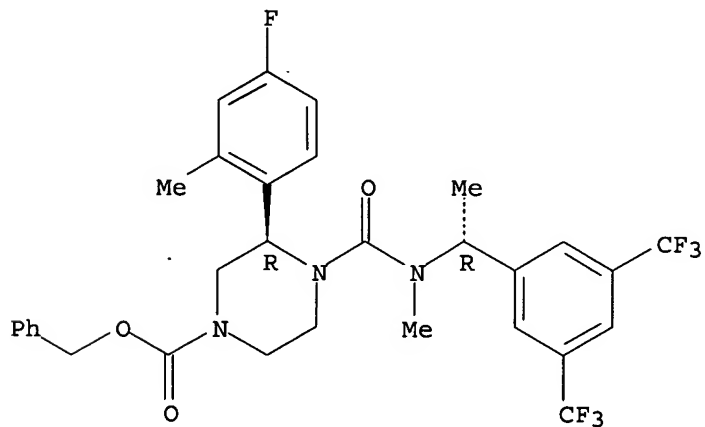
Absolute stereochemistry.



RN 334477-06-4 CAPLUS

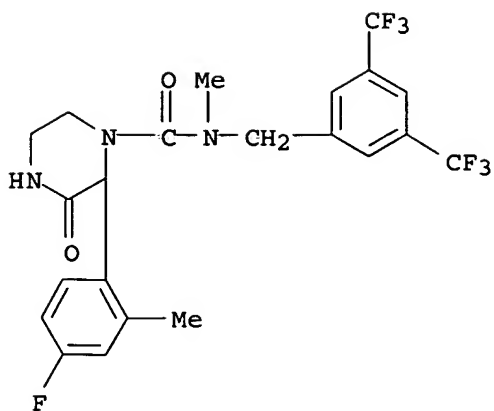
CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester, (3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



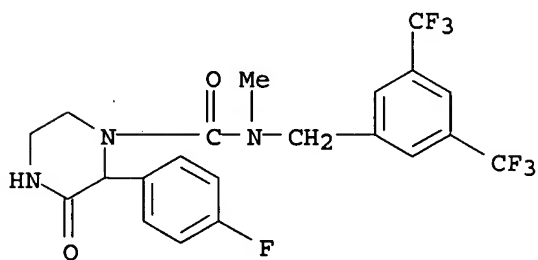
RN 334477-11-1 CAPLUS

CN 1-Piperazinecarboxamide, N-[[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo- (9CI) (CA INDEX NAME)



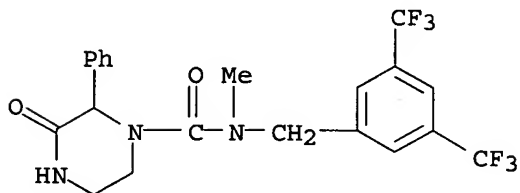
RN 334477-12-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluorophenyl)-N-methyl-3-oxo- (9CI) (CA INDEX NAME)



RN 334477-13-3 CAPLUS

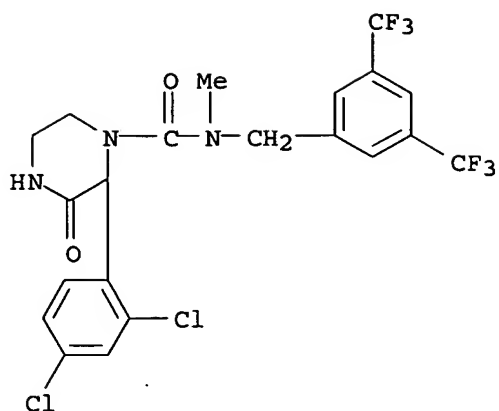
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-3-oxo-2-phenyl- (9CI) (CA INDEX NAME)



RN 334477-14-4 CAPLUS

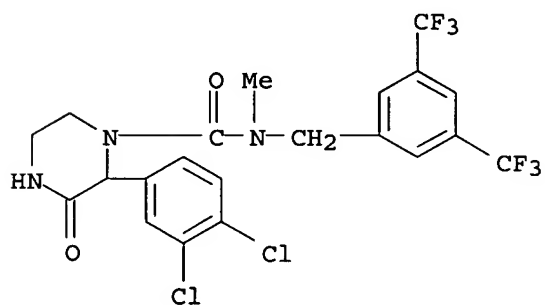
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(2,4-dichlorophenyl)-N-methyl-3-oxo- (9CI) (CA INDEX NAME)

10/089964



RN 334477-15-5 CAPLUS

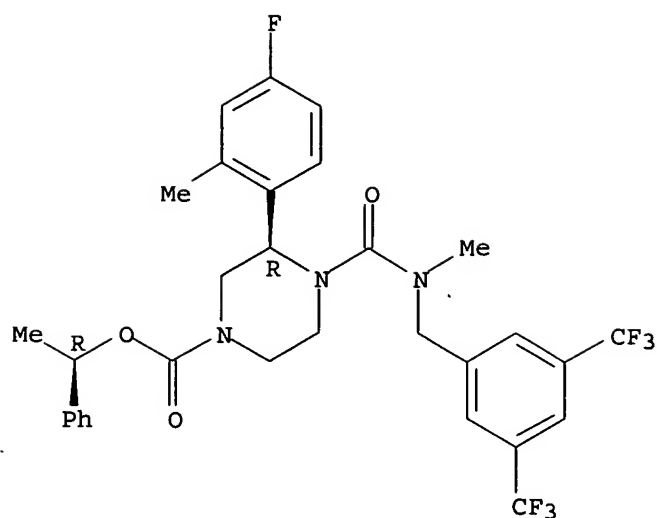
CN 1-Piperazinecarboxamide, N-[[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(3,4-dichlorophenyl)-N-methyl-3-oxo- (9CI) (CA INDEX NAME)



RN 334477-16-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1R)-1-phenylethyl ester, (3R)- (9CI) (CA INDEX NAME)

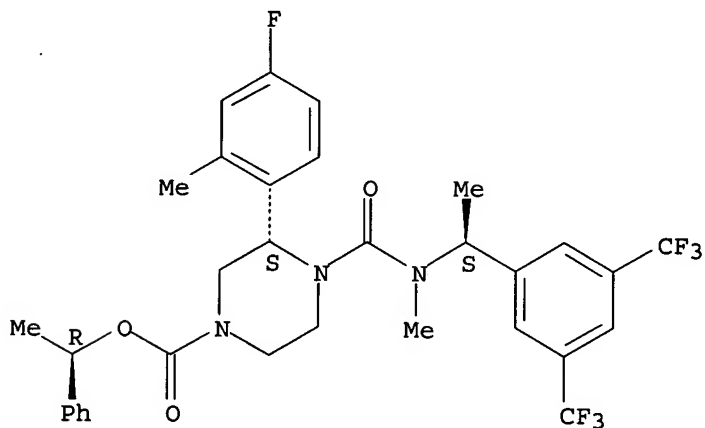
Absolute stereochemistry.



RN 334477-17-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1R)-1-phenylethyl ester, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

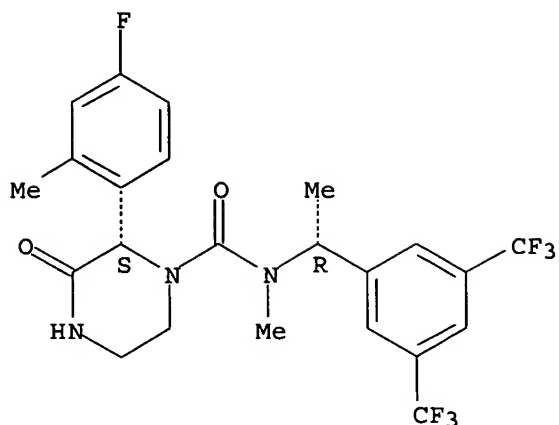


RN 334477-19-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo-, (2S)-(9CI) (CA INDEX NAME)

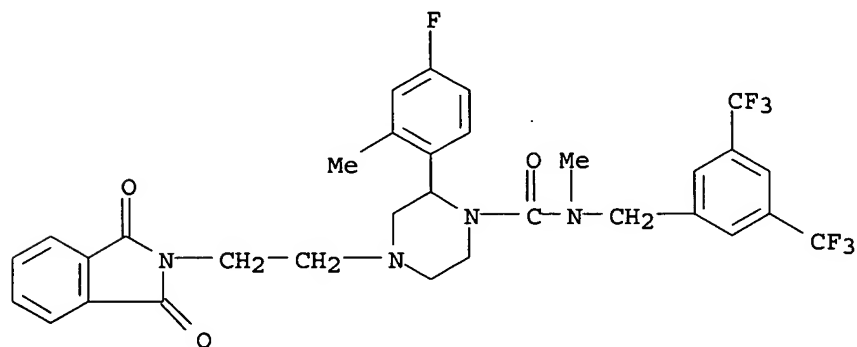
Absolute stereochemistry.

10/089964



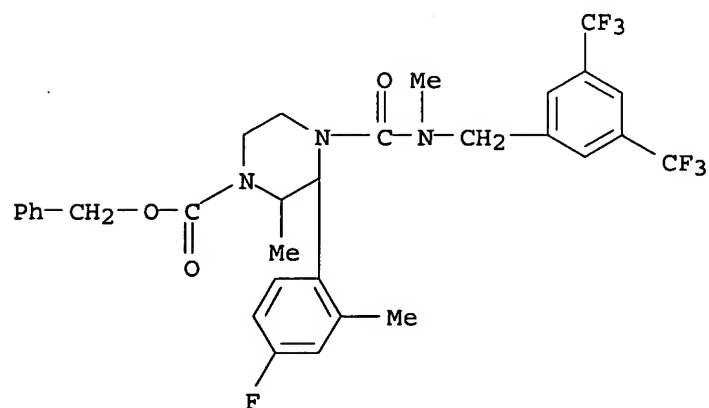
RN 334477-20-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[[[3,5-bis(trifluoromethyl)phenyl]methyl]-4-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 334477-24-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

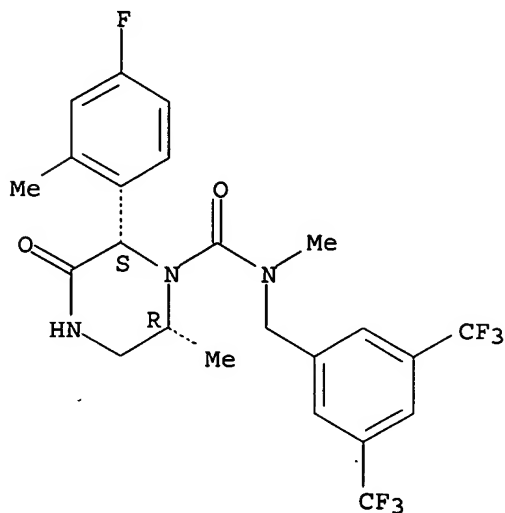


10/089964

RN 334477-27-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N,6-dimethyl-3-oxo-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

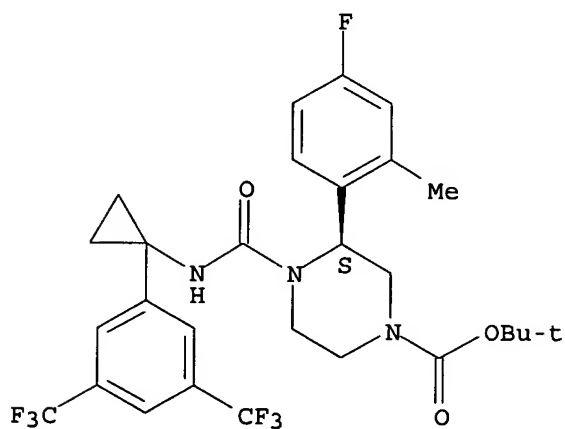
Relative stereochemistry.



RN 334477-31-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]cyclopropyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

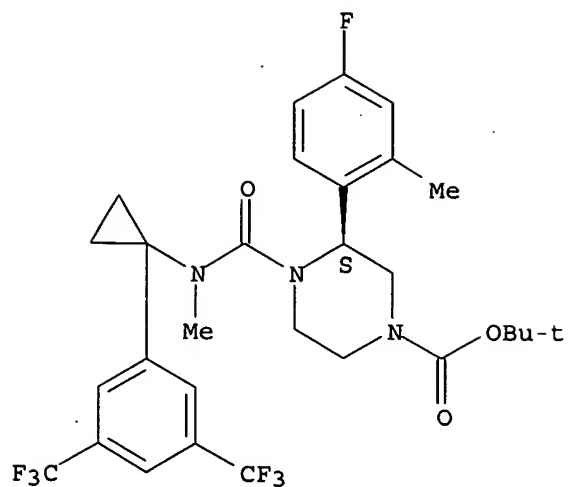
Absolute stereochemistry.



RN 334477-32-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]cyclopropyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

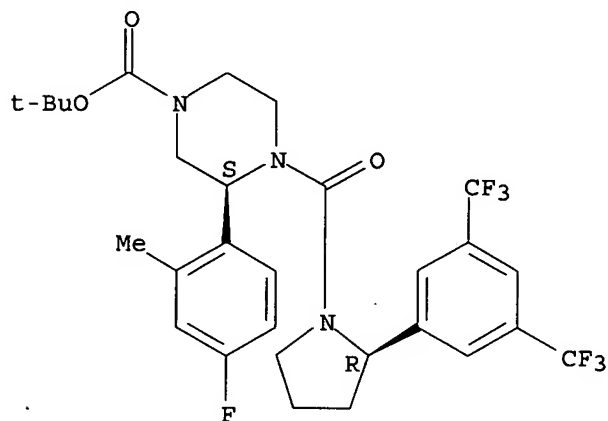
Absolute stereochemistry.



RN 334477-37-1 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(2R)-2-[3,5-bis(trifluoromethyl)phenyl]-1-pyrrolidinyl]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

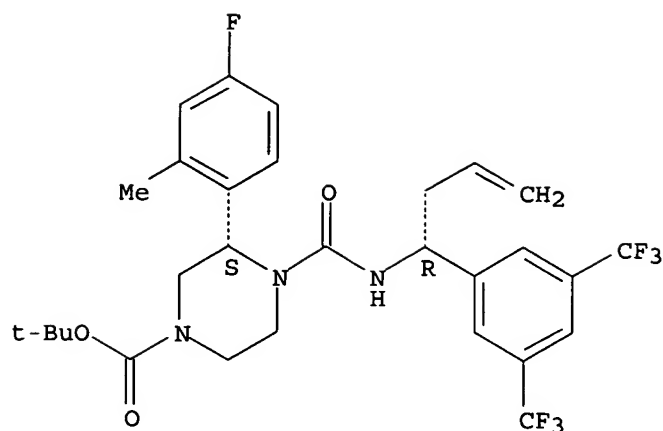


RN 334477-39-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

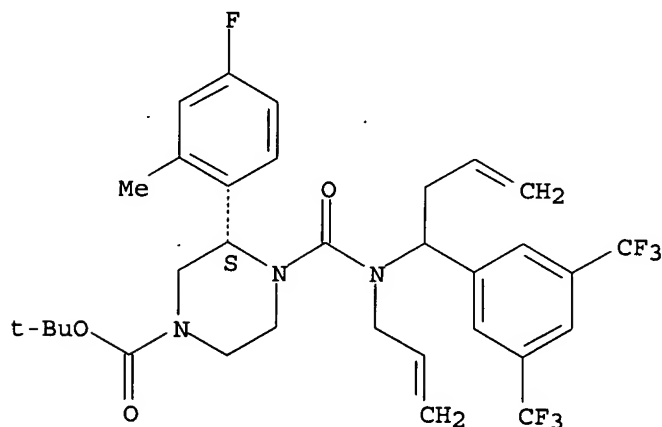
10/089964



RN 334477-40-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]-2-propenylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

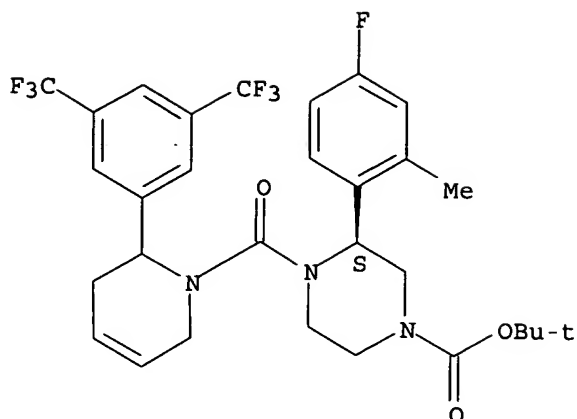


RN 334477-41-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[2-[3,5-bis(trifluoromethyl)phenyl]-3,6-dihydro-1(2H)-pyridinyl]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

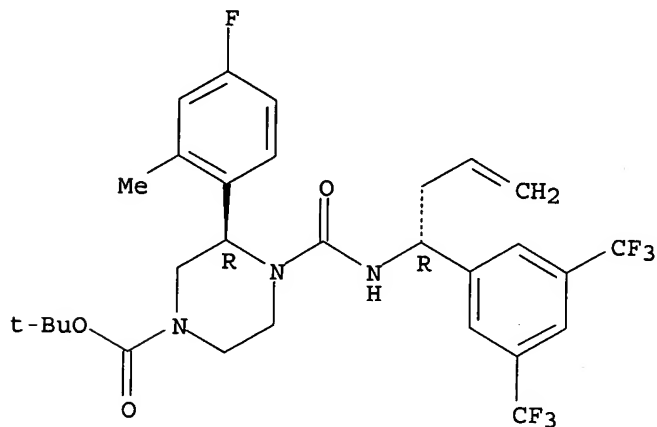
10/089964



RN 334477-43-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

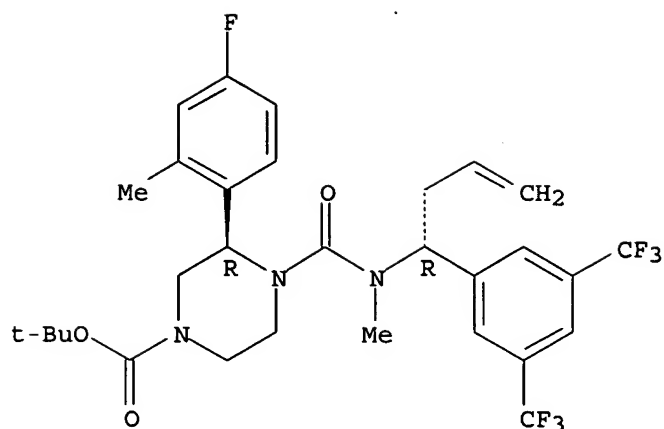


RN 334477-44-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

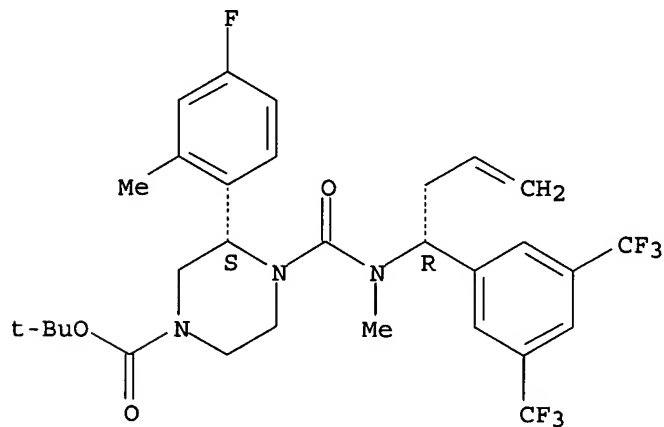
10/089964



RN 334477-45-1 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)-rel- (9CI) (CA INDEX NAME)

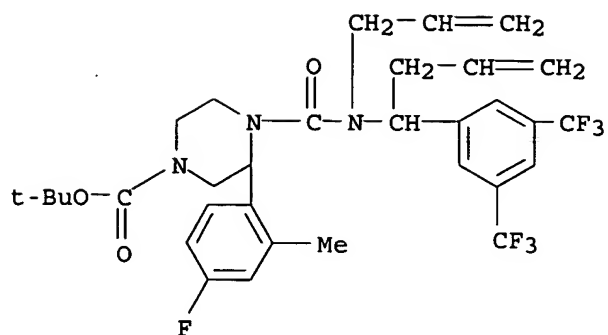
Relative stereochemistry.



RN 334477-46-2 CAPLUS

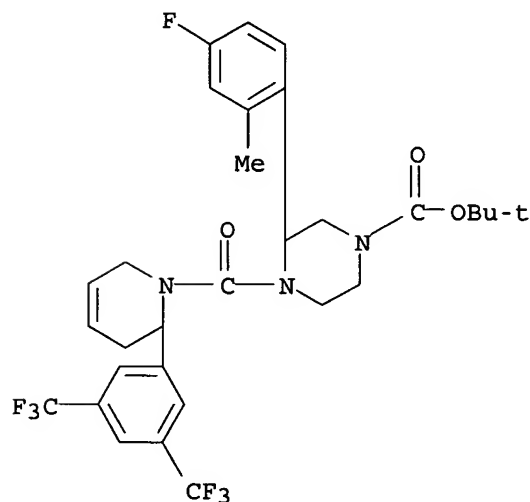
CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]-2-propenylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

10/089964



RN 334477-47-3 CAPLUS

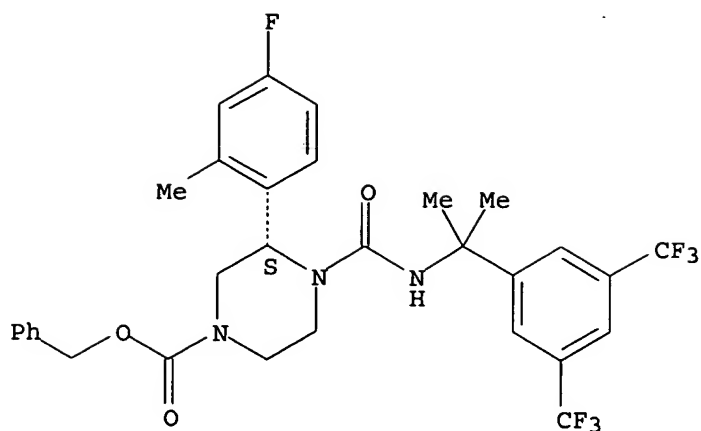
CN 1-Piperazinecarboxylic acid, 4-[[2-[3,5-bis(trifluoromethyl)phenyl]-3,6-dihydro-1(2H)-pyridinyl]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 334477-50-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]-1-methylethyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester, (3S)-(9CI) (CA INDEX NAME)

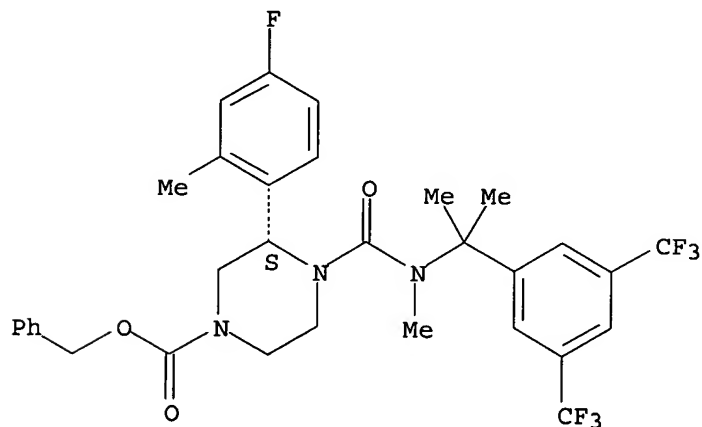
Absolute stereochemistry.



RN 334477-51-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]-1-methylethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

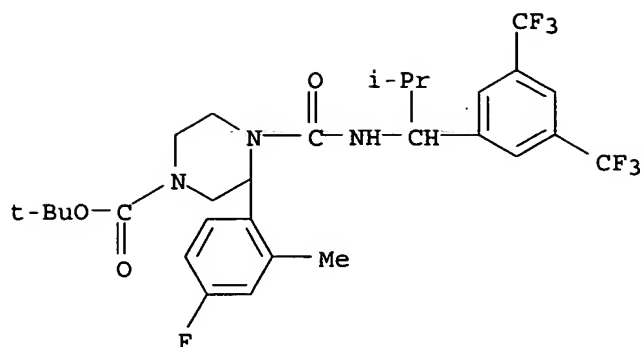
Absolute stereochemistry.



RN 334477-54-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

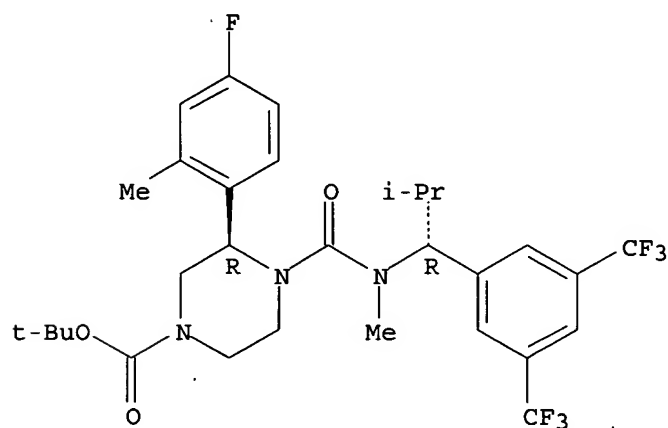
10/089964



RN 334477-55-3 CAPLUS

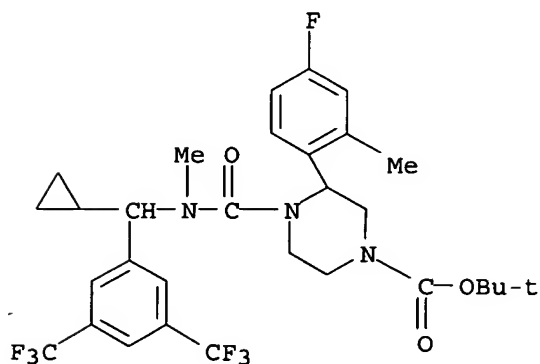
CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 334477-58-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]cyclopropylmethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

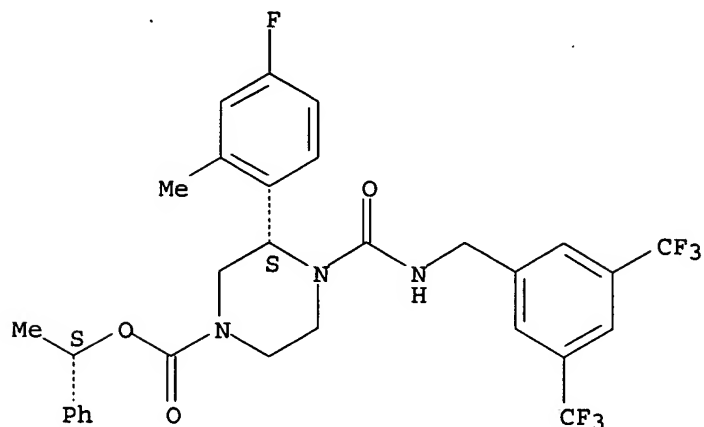


10/089964

RN 334477-66-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1S)-1-phenylethyl ester, (3S)- (9CI) (CA INDEX NAME)

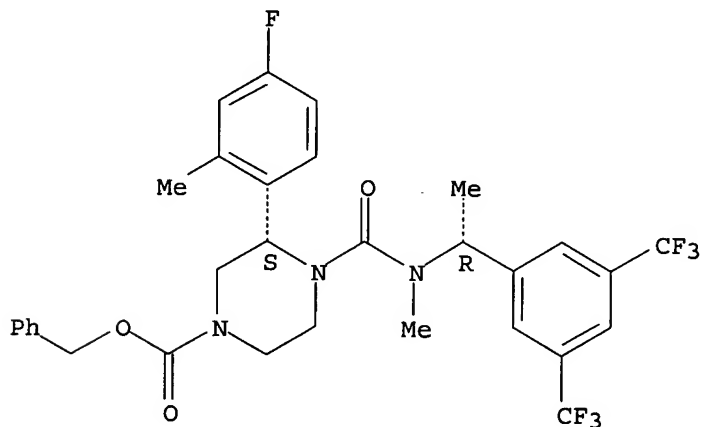
Absolute stereochemistry.



RN 334477-67-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, phenylmethyl ester, (3S)-rel- (9CI) (CA INDEX NAME)

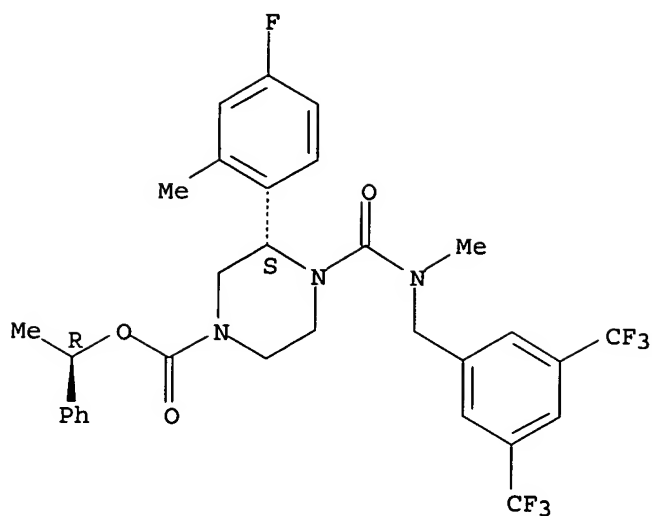
Relative stereochemistry.



RN 334477-70-2 CAPLUS

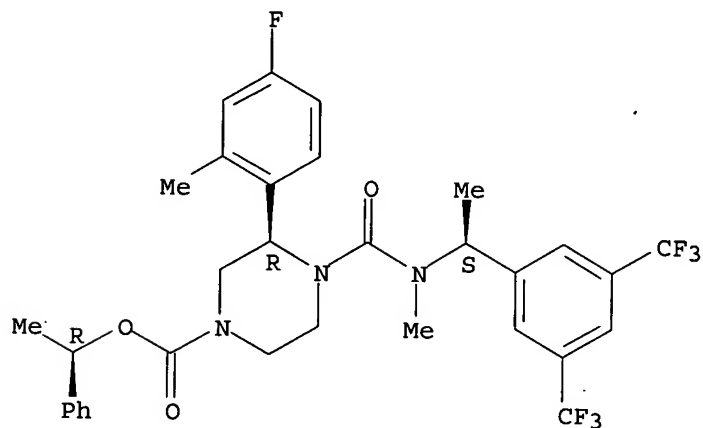
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1R)-1-phenylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 334477-71-3 CAPLUS
 CN 1-Piperazinecarboxylic acid, 4-[[[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, (1R)-1-phenylethyl ester, (3R)- (9CI) (CA INDEX NAME)

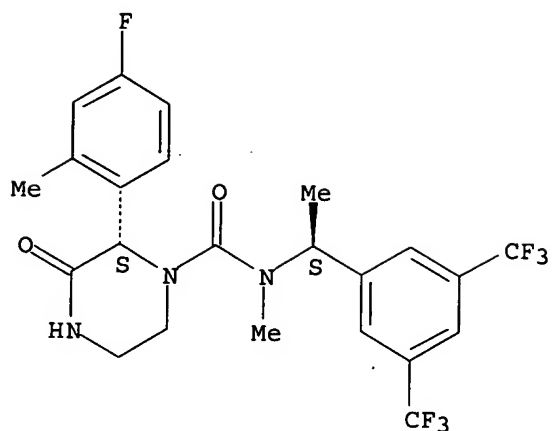
Absolute stereochemistry.



RN 334477-73-5 CAPLUS
 CN 1-Piperazinecarboxamide, N-[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-3-oxo-, (2S)- (9CI) (CA INDEX NAME)

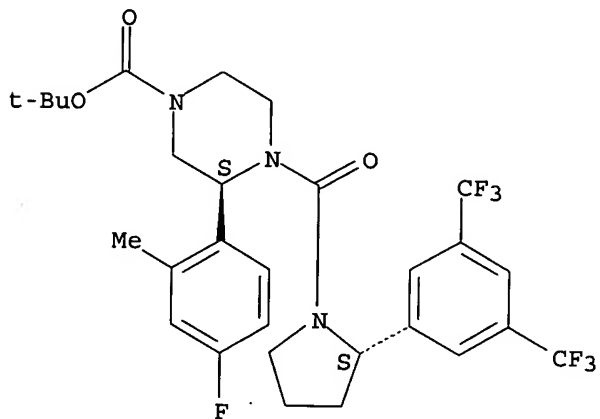
Absolute stereochemistry.

10/089964



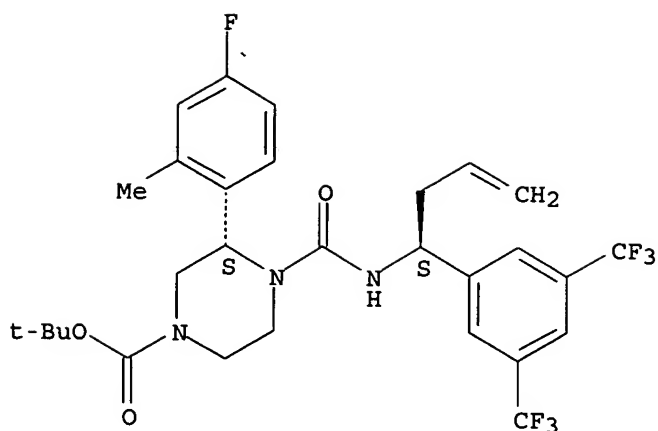
RN 334477-77-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[(2S)-2-[3,5-bis(trifluoromethyl)phenyl]-1-pyrrolidinyl]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 334477-78-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[(1S)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

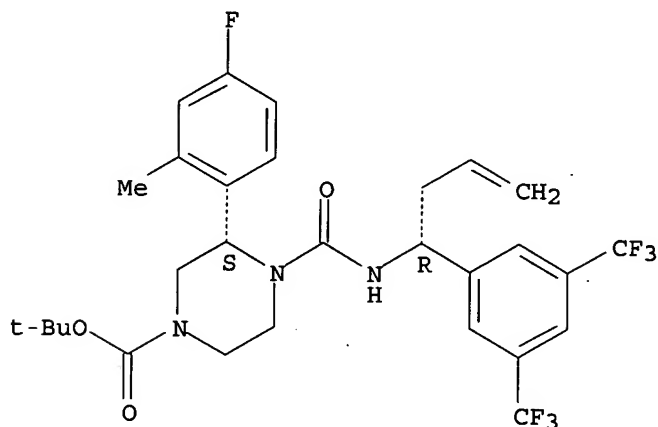
Absolute stereochemistry.



RN 334477-79-1 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-3-butenyl]amino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

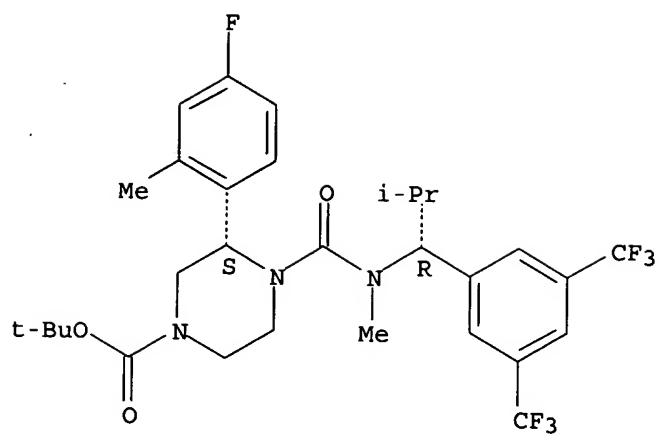


RN 334477-80-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]-2-methylpropyl]methylamino]carbonyl]-3-(4-fluoro-2-methylphenyl)-, 1,1-dimethylethyl ester, (3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

10/089964



10/089964

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 1989:594366 CAPLUS

DN 111:194366

TI Synthesis and biological activity of a series of piperazine-2,3-dione containing penicillins and 6.alpha.-formamidopenicillins. I. Derivatives substituted at C(5) or C(6) of the piperazine ring

AU Davies, David T.; Harrington, Frank P.; Knott, Sarah J.; Southgate, Robert

CS Chemother. Res. Cent., Beecham Pharm., Betchworth/Surrey, RH3 7AJ, UK

SO Journal of Antibiotics (1989), 42(3), 367-73

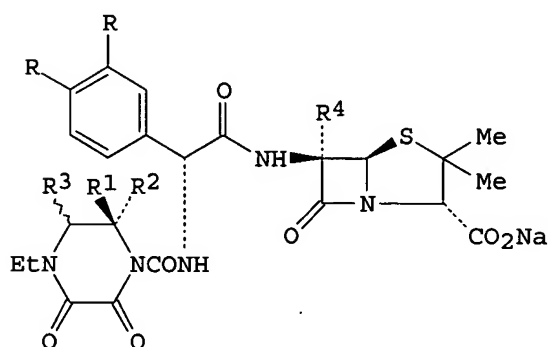
CODEN: JANTAJ; ISSN: 0021-8820

DT Journal

LA English

OS CASREACT 111:194366

GI



I

AB Title compds. I (R = H, OAc; R1 - R3 = H, Me, Ph; R4 = H, NHCHO) were prepd. The products had bactericidal activity, but offered no advantage over I (R - R3 = H, R4 = H, NHCHO).

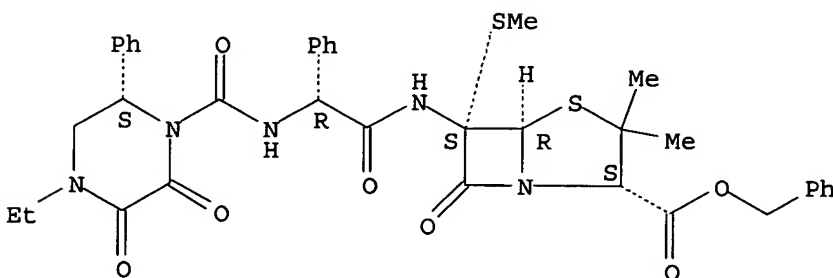
IT 123361-19-3P 123361-31-9P 123409-99-4P
123410-14-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and aminolysis of)

RN 123361-19-3 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-6-(methylthio)-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.alpha.,6[S*(R*)]]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

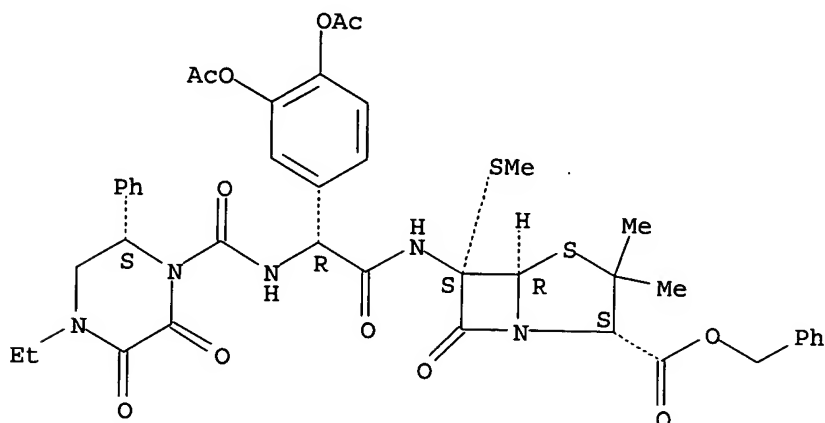


RN 123361-31-9 CAPLUS

10/089964

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-3,3-dimethyl-6-(methylthio)-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.alpha.,6[S*(R*)]]]- (9CI)
(CA INDEX NAME)

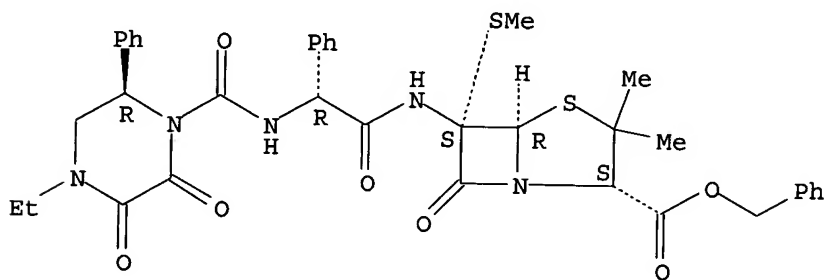
Absolute stereochemistry.



RN 123409-99-4 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-6-(methylthio)-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.alpha.,6[S*(S*)]]]- (9CI) (CA INDEX NAME)

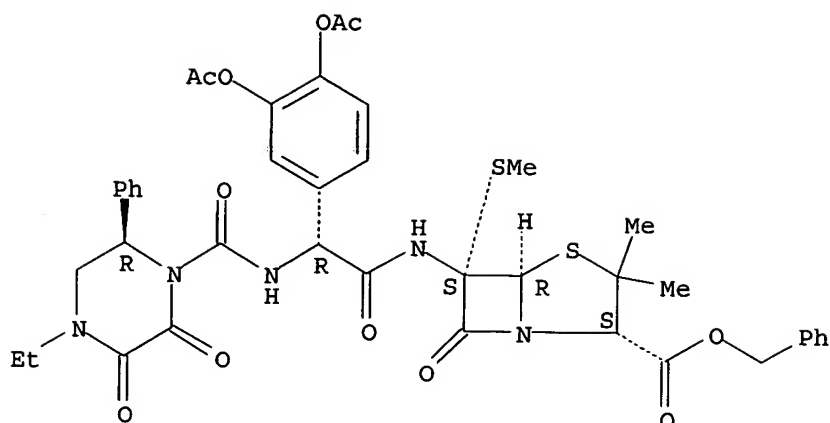
Absolute stereochemistry.



RN 123410-14-0 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-3,3-dimethyl-6-(methylthio)-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.alpha.,6[S*(S*)]]]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



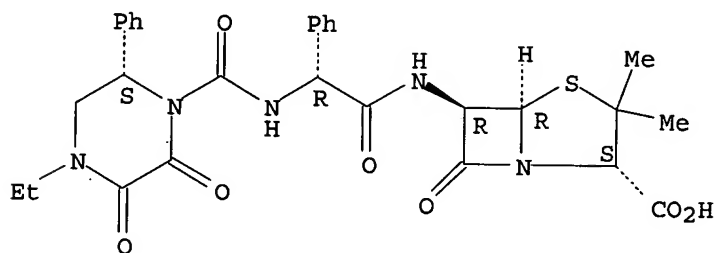
IT 123361-17-1P 123361-27-3P 123361-35-3P
 123409-96-1P 123409-97-2P 123410-04-8P
 123410-08-2P 123410-17-3P 123410-18-4P
 123482-37-1P 123482-41-7P 123482-44-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. and bactericidal activity of)

RN 123361-17-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

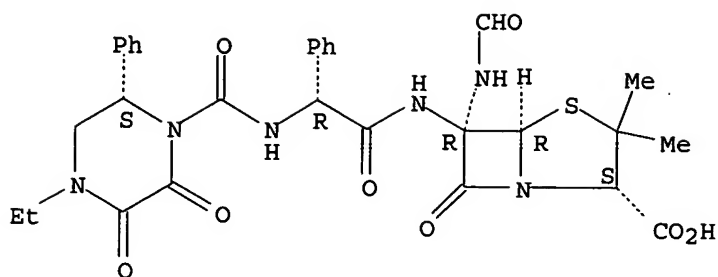


● Na

RN 123361-27-3 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

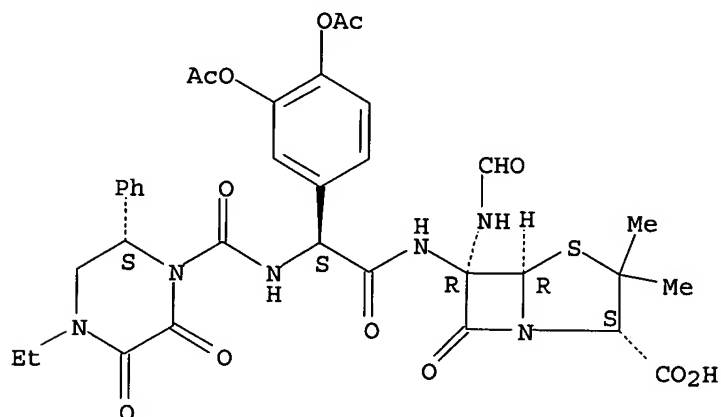


● Na

RN 123361-35-3 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.[R*(R*)]]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



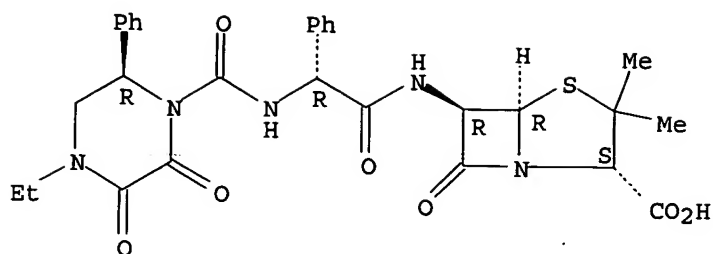
● Na

RN 123409-96-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.[S*(S*)]]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964

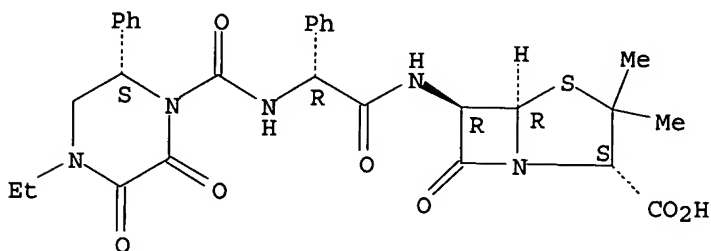


● Na

RN 123409-97-2 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]- (9CI) (CA INDEX NAME)

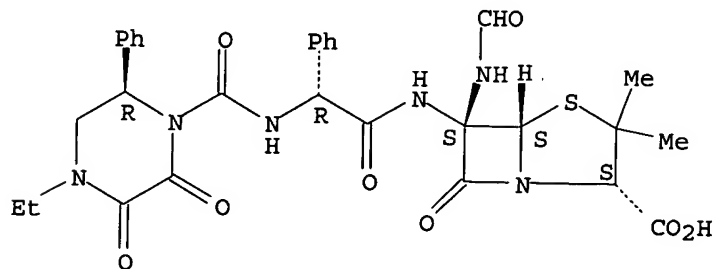
Absolute stereochemistry.



RN 123410-04-8 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.beta.,6.alpha.[S*(S*)]]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



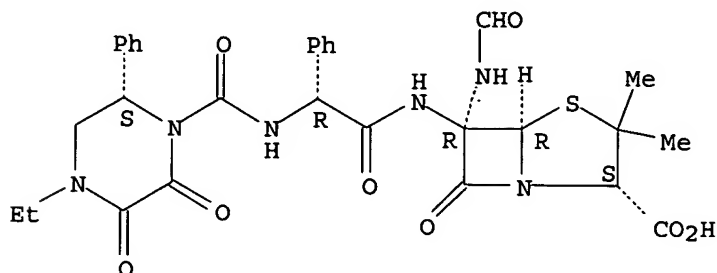
Na

RN 123410-08-2 CAPLUS

10/089964

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]- (9CI) (CA INDEX NAME)

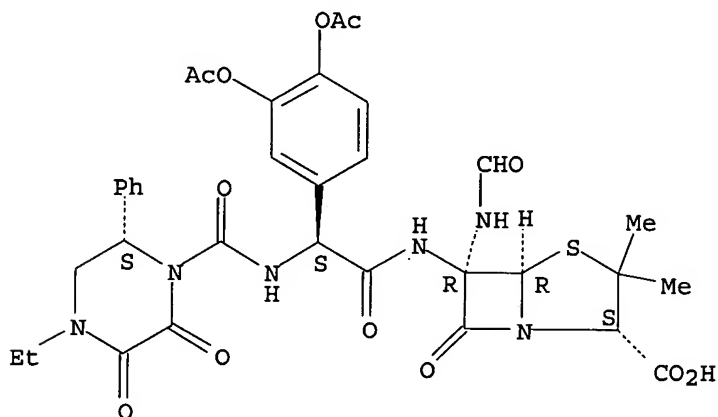
Absolute stereochemistry.



RN 123410-17-3 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[R*(R*)]]]- (9CI) (CA INDEX NAME)

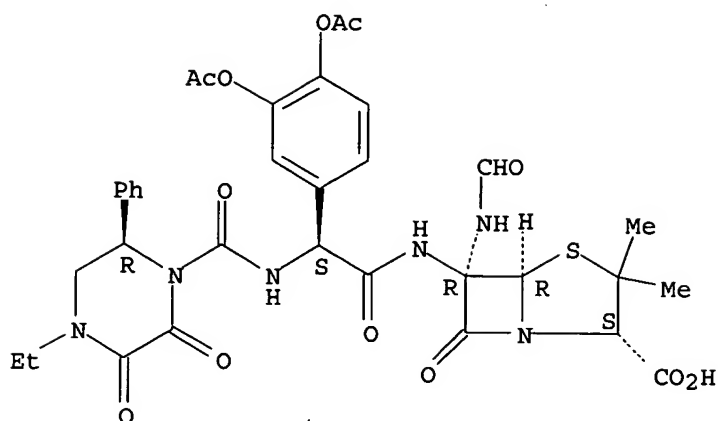
Absolute stereochemistry.



RN 123410-18-4 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[R*(S*)]]]- (9CI) (CA INDEX NAME)

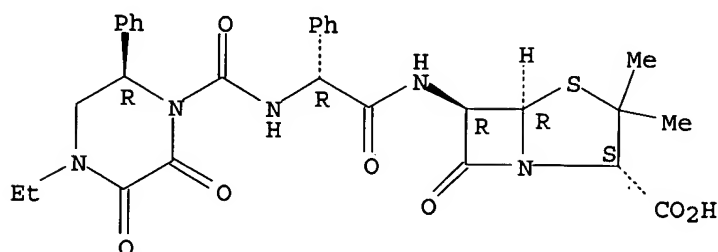
Absolute stereochemistry.



RN 123482-37-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[S*(S*)]]]- (9CI) (CA INDEX NAME)

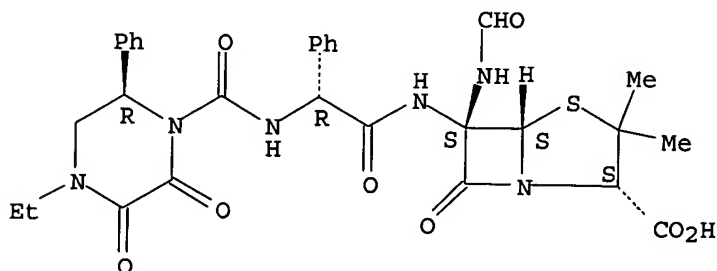
Absolute stereochemistry.



RN 123482-41-7 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.beta.,6.alpha.[S*(S*)]]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



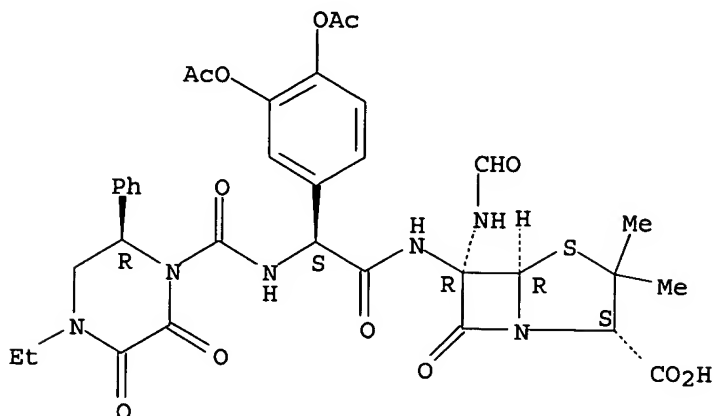
RN 123482-44-0 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-

10/089964

piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.[R*(S*)]]]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



● Na

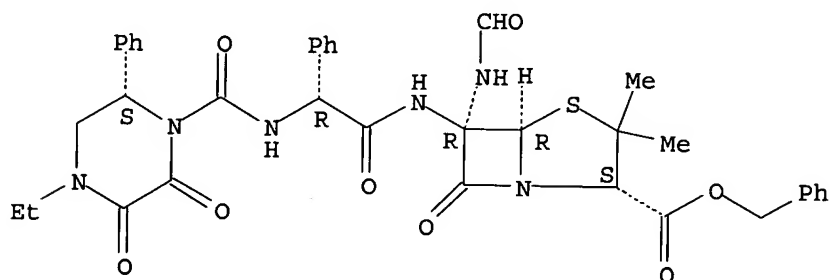
IT 123361-23-9P 123361-33-1P 123410-02-6P
123410-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and hydrogenolysis of)

RN 123361-23-9 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]- (9CI) (CA INDEX NAME)

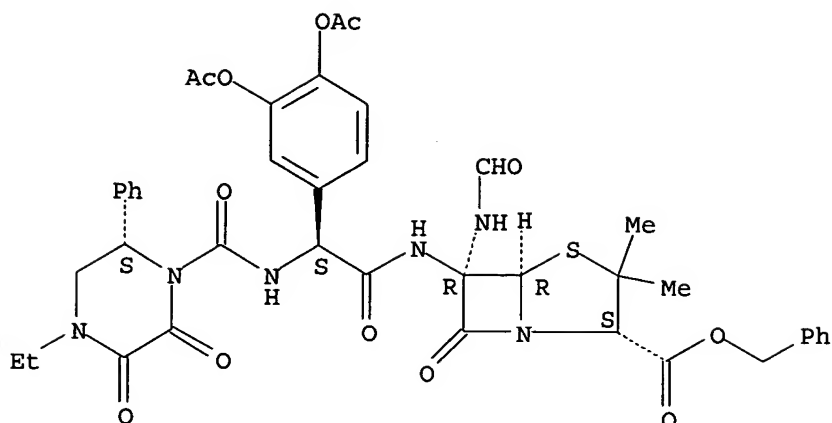
Absolute stereochemistry.



RN 123361-33-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.beta.[R*(R*)]]]- (9CI)
(CA INDEX NAME)

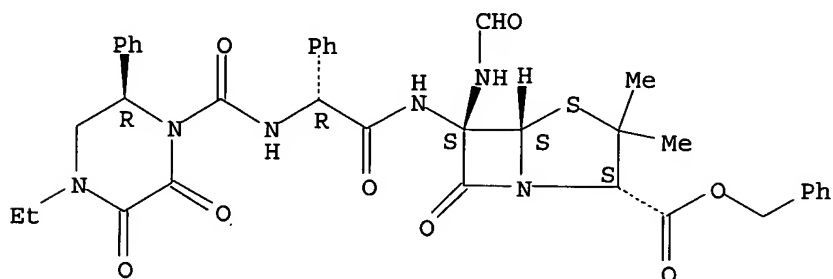
Absolute stereochemistry.



RN 123410-02-6 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.beta.,6.alpha.[S*(S*)]]]- (9CI) (CA INDEX NAME)

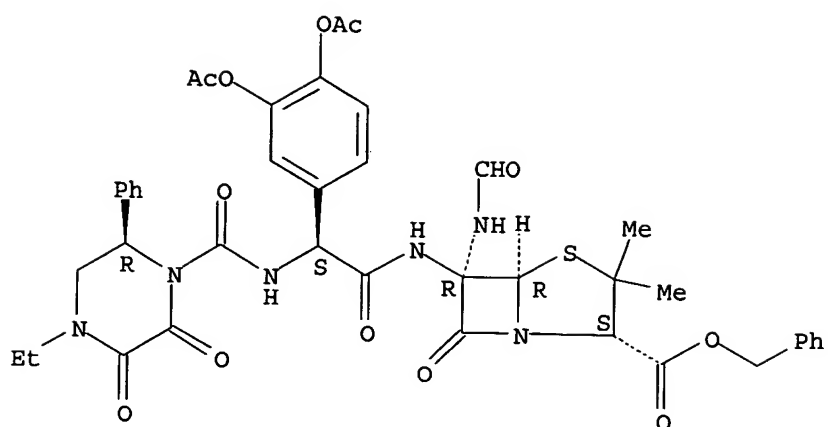
Absolute stereochemistry.



RN 123410-15-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[3,4-bis(acetyloxy)phenyl][[(4-ethyl-2,3-dioxo-6-phenyl-1-piperazinyl)carbonyl]amino]acetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.beta.[R*(S*)]]]- (9CI) (CA INDEX NAME)

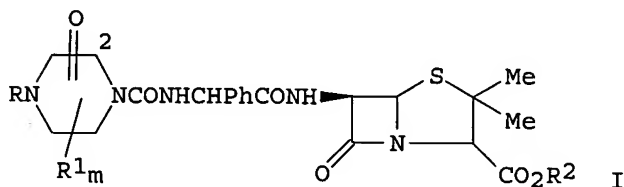
Absolute stereochemistry.



10/089964

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS
AN 1983:71807 CAPLUS
DN 98:71807
TI Penicillins.
PA Toyama Chemical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 57118587	A2	19820723	JP 1981-188407	19811126
PRAI	JP 1981-188407		19811126		
OS	CASREACT 98:71807				
GI					



AB Forty-eight penicillin derivs. [d-(-)-I; R = H, alkyl, alkenyl, acyl, aroyl, etc.; R₁ = H, Me, Ph, etc.; R₂ = H, Na; m = 1, 2], effective bactericides at 0.4-100 .mu.g/mL, were prepd. Thus, 3.71 g Me₃SiCl was refluxed with 2.5 g 1-acetyl-3-oxopiperazine and 3.45 g Et₃N in dioxane, Et₃N.HCl filtered, and the filtrate treated with 1.8 g COCl₂ at -30.degree. to -40.degree. and room temp. to give 3.5 g 4-acetyl-2-oxo-1-piperazinecarbonyl chloride, which (900 mg) was treated with 1.0 g 6-[d-(-)-.alpha.-amino-.alpha.-phenylacetamidol]penicillanic acid in 80% aq. THF at 0.degree. and pH 8.0-8.5, and the mixt. kept at pH 7.5-8.0 and 5-10.degree. to give 94% I (R = Ac, R₁ = H, R₂ = Na, O at 2-position).

IT 59703-75-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal activity of)

RN 59703-75-2 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[[[(3-oxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964

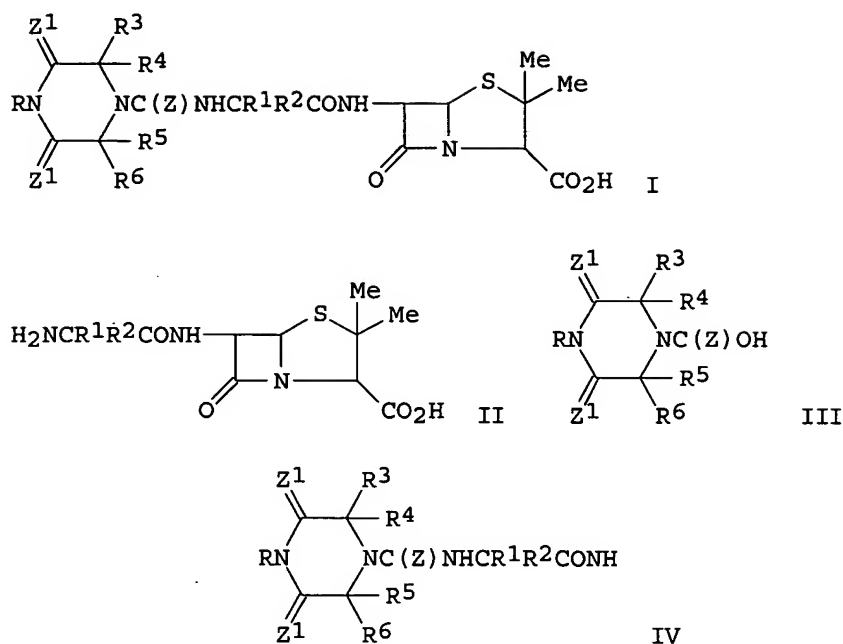
L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS
 AN 1976:463059 CAPLUS
 DN 85:63059
 TI Penicillins
 IN Saikawa, Isamu; Takano, Shuntaro; Yoshida, Chosaku; Takashima, Okuta;
 Momoi, Kaishu; Kuroda, Seietsu; Komatsu, Miwako; Yasuda, Takashi; Kodama,
 Yutaka
 PA Toyama Chemical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 51039687	A2	19760402	JP 1974-109954	19740926
	AU 7580431	A1	19761028	AU 1975-80431	19750423
	US 4087424	A	19780502	US 1975-571479	19750424
	IL 47168	A1	19790725	IL 1975-47168	19750424
	IL 53485	A1	19790930	IL 1975-53485	19750424
	GB 1508062	A	19780419	GB 1975-17557	19750428
	GB 1508064	A	19780419	GB 1977-15360	19750428
	GB 1508063	A	19780419	GB 1977-15363	19750428
	DE 2519400	A1	19760304	DE 1975-2519400	19750430
	DE 2519400	B2	19810521		
	DE 2519400	C3	19820211		
	DE 2559932	C2	19830421	DE 1975-2559932	19750430
	DE 2560239	C2	19841011	DE 1975-2560239	19750430
	CA 1061331	A1	19790828	CA 1975-226043	19750501
	FR 2269937	A1	19751205	FR 1975-14159	19750506
	FR 2269937	B1	19790615		
	CH 605995	A	19781013	CH 1975-5847	19750506
	FI 7501340	A	19751110	FI 1975-1340	19750507
	FI 63760	B	19830429		
	FI 63760	C	19830810		
	DK 7502019	A	19751110	DK 1975-2019	19750507
	DK 151338	B	19871123		
	DK 151338	C	19880718		
	AT 7503511	A	19770315	AT 1975-3511	19750507
	AT 340046	B	19771125		
	DD 117882	C	19760205	DD 1975-185922	19750508
	HU 169633	P	19761228	HU 1975-T01002	19750508
	SE 7505392	A	19751223	SE 1975-5392	19750509
	SE 431457	B	19840206		
	SE 431457	C	19840517		
	GB 1508071	A	19780419	GB 1976-2002	19760119
	US 4112090	A	19780905	US 1976-654060	19760130
	US 4110327	A	19780829	US 1976-732860	19761015
	FR 2320295	A1	19770304	FR 1976-31895	19761022
	FR 2320295	B1	19801107		
	IN 145443	A	19781014	IN 1976-CA2121	19761127
	IN 145444	A	19781014	IN 1976-CA2122	19761127
	US 4410522	A	19831018	US 1977-841608	19771012
	CH 616939	A	19800430	CH 1977-16075	19771227
	FI 62833	B	19821130	FI 1978-330	19780201
	FI 62833	C	19830310		
	US 4219554	A	19800826	US 1978-915873	19780615
	CA 1078384	A1	19800527	CA 1978-308161	19780726
	SE 7808204	A	19780727	SE 1978-8204	19780727
	SE 435062	B	19840903		

10/089964

SE 435062	C	19841213		
DK 7901049	A	19790314	DK 1979-1049	19790314
DK 149950	B	19861103		
DK 149950	C	19870928		
US 4379152	A	19830405	US 1979-39904	19790517
US 4327097	A	19820427	US 1979-47818	19790612
DK 8000958	A	19800306	DK 1980-958	19800306
DK 151958	B	19880118		
DK 151958	C	19880718		
FI 8100165	A	19810121	FI 1981-165	19810121
FI 65780	B	19840330		
FI 65780	C	19840710		
FI 8100468	A	19810216	FI 1981-468	19810216
FI 62834	B	19821130		
FI 62834	C	19830310		
PRAI JP 1974-50663		19740509		
JP 1974-52254		19740513		
JP 1974-60787		19740531		
JP 1974-91996		19740813		
JP 1974-109954		19740926		
JP 1974-142499		19741213		
JP 1975-142499		19750327		
JP 1975-37027		19750327		
JP 1975-37207		19750327		
IL 1975-47168		19750424		
US 1975-571479		19750424		
GB 1975-17557		19750428		
IN 1975-CA852		19750428		
CH 1975-5847		19750506		
DK 1975-2019		19750507		
FI 1975-1340		19750507		
US 1976-654060		19760130		
FI 1978-330		19780201		
US 1978-915873		19780615		

GI



AB Penicillins I (R = H, halo, OH, NO₂, cyano, alkyl, acyloxyalkyl, aryl, cycloalkyl, etc.; R₁ = alkyl, cycloalkyl, cycloalkenyl, cycloalkadienyl, aryl, aralkyl, alkylthioalkyl, aryloxy, heterocyclyls; R₂ = H; R₁R₂ may form a cycloalkyl, cycloalkenyl, cycloalkadienyl ring; R₃-R₆ = H, halo, CO₂H, alkyl, acyloxyalkyl, aryl, etc.; R₃R₄ or R₅R₆ may form a cycloalkyl, cycloalkenyl, cycloalkadienyl ring; Z, Z₁ = O, S), and their salts and esters were prepd. by reaction of the amineacetamidopenicillanic acids II or their derivs. with the piperazines or their III reactive derivs. or by reaction of 6-aminopenicillanic acid or their derivs. with the piperazinecarboxamidoacetic acids IV or their reactive derivs. I are antibiotics with a wide antibacterial spectrum. Thus, 244 mg 2,2-pentamethylene-3,5-dioxo-1-piperazinylcarbonyl chloride in THF was treated at 0.degree. with 350 mg D(-)-.alpha.-aminobenzylpenicillin in 80% aq. THF and the mixt. adjusted to pH 8.0-8.5 with Et₃N and then at 5-10.degree. and pH 7.5-8.0 to give 500 mg D(-)-.alpha.-(2,2-pentamethylene-3,5-dioxo-1-piperazinylcarboxamido)benzylpenicillin. Also, prepd. were D(-)-.alpha.-(4-benzyl-2,2-pentamethylene-3,5-dioxo-1-piperazinecarboxamido)-, D(-)-.alpha.-(4-.beta.,.beta.,.beta.-trichloroethoxycarbonyl-2,2-pentamethylene-3,5-dioxo-1-piperazinecarboxamido)-, D(-)-.alpha.-(3,5-dioxopiperazinecarboxamido)-, D(-)-.alpha.-(2-methyl-2-phenyl-3,5-dioxopiperazinecarboxamido)-, and D(2-)-.alpha.-(4-benzyl-2-methyl-2-phenyl-3,5-dioxopiperazinecarboxamido)benzylpenicillins.

IT 59703-79-6P 59703-82-1P

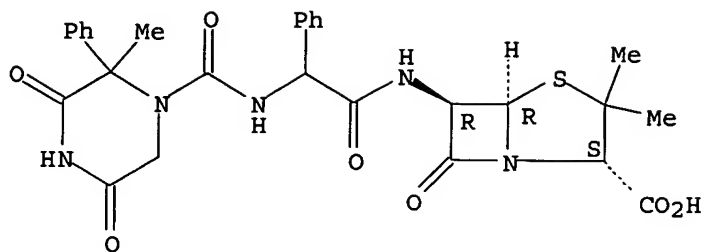
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59703-79-6 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[[(2-methyl-3,5-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-7-oxo-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

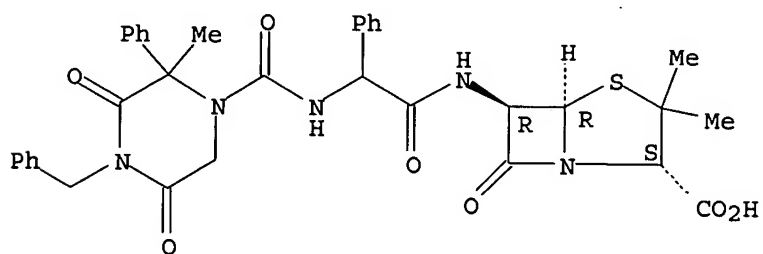
10/089964



RN 59703-82-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[[2-methyl-3,5-dioxo-2-phenyl-4-(phenylmethyl)-1-piperazinyl]carbonyl]amino]phenylacetyl]amino]-7-oxo-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

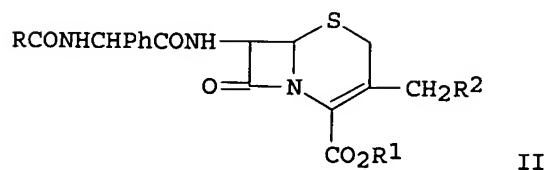
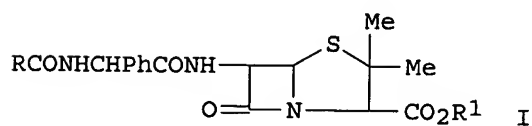


10/089964

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS
 AN 1976:433052 CAPLUS
 DN 85:33052
 TI Penicillin and cephalosporin derivatives
 IN Saikawa, Isamu; Takano, Shuntaro; Yoshida, Chosaku; Takashima, Okuta;
 Momonoi, Kaishu; Kuroda, Seietsu; Komatsu, Miwako; Yasuda, Takashi;
 Kodama, Yutaka
 PA Toyama Chemical Co., Ltd., Japan
 SO Ger. Offen., 237 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2519400	A1	19760304	DE 1975-2519400	19750430
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	DE 2519400	C3	19820211		
	JP 50148378	A2	19751127	JP 1974-50663	19740509
	JP 50148380	A2	19751127	JP 1974-52254	19740513
	JP 50151891	A2	19751206	JP 1974-60787	19740531
	JP 51023284	A2	19760224	JP 1974-91996	19740813
	JP 51039687	A2	19760402	JP 1974-109954	19740926
	JP 51070788	A2	19760618	JP 1974-142499	19741213
	JP 51113890	A2	19761007	JP 1975-37207	19750327
	AT 7608289	A	19771215	AT 1976-8289	19761108
	ES 454266	A1	19771216	ES 1976-454266	19761215
	ES 454267	A1	19771216	ES 1976-454267	19761215
	US 4379152	A	19830405	US 1979-39904	19790517
PRAI	JP 1974-50663		19740509		
	JP 1974-52254		19740513		
	JP 1974-60787		19740531		
	JP 1974-91996		19740813		
	JP 1974-109954		19740926		
	JP 1974-142499		19741213		
	JP 1975-37207		19750327		
	AT 1975-3511		19750507		
	US 1976-654060		19760130		
	US 1978-915873		19780615		

GI



AB Acylaminobenzylpenams I and -cephems II (R = substituted oxopiperazino; R1

10/089964

= H, Na, ester; R2 = H, OAc, heterocyclic thiol) (164 compds.) were prepd. by acylating aminobenzylpenams and -cephems. Thus 1-acetyl-3-oxopiperazine was treated with COCl2 and used to acylate ampicillin to I (R = 4-acetyl-2-oxopiperazino, R1 = Na).

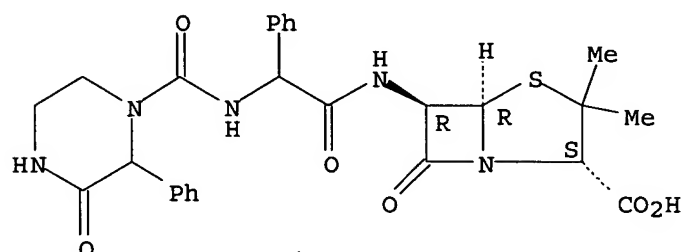
IT 59703-75-2P 59703-79-6P 59703-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 59703-75-2 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-7-oxo-6-[[[(3-oxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

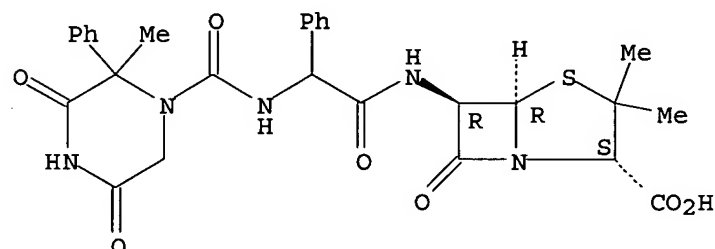
Absolute stereochemistry.



RN 59703-79-6 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[[(2-methyl-3,5-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-7-oxo-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

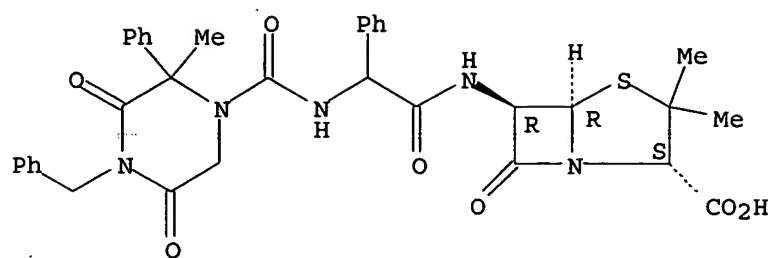


RN 59703-82-1 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 3,3-dimethyl-6-[[[(2-methyl-3,5-dioxo-2-phenyl-4-(phenylmethyl)-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-7-oxo-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/089964



10/089964

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	31.39	188.95
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.91	-3.91

FILE 'CAOLD' ENTERED AT 12:02:18 ON 14 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 11:54:21 ON 14 JUL 2003)

FILE 'REGISTRY' ENTERED AT 11:54:29 ON 14 JUL 2003

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L3 154 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:56:26 ON 14 JUL 2003

L4 6 S L3

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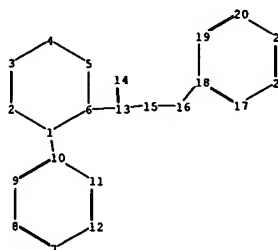
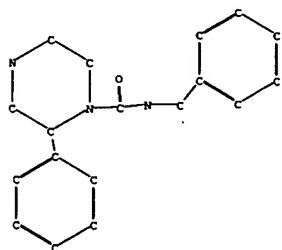
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CA SUBSCRIBER PRICE	0.00	-3.91

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:02:36 ON 14 JUL 2003



chain nodes :

13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 17 18 19 20 21 22

ring/chain nodes :

15 16

chain bonds :

1-10 6-13 13-14 13-15 16-18

ring/chain bonds :

15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-18 17-22 18-19
19-20 20-21 21-22

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-13 13-14 13-15 15-16

exact bonds :

1-10 16-18

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12 17-18 17-22 18-19 19-20 20-21 21-22

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom

10/089964

=> s l1

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SAMPLE SCREEN SEARCH COMPLETED - 53 TO ITERATE

100.0% PROCESSED 53 ITERATIONS
SEARCH TIME: 00.00.01

5 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 624 TO 1496
PROJECTED ANSWERS: 5 TO 234

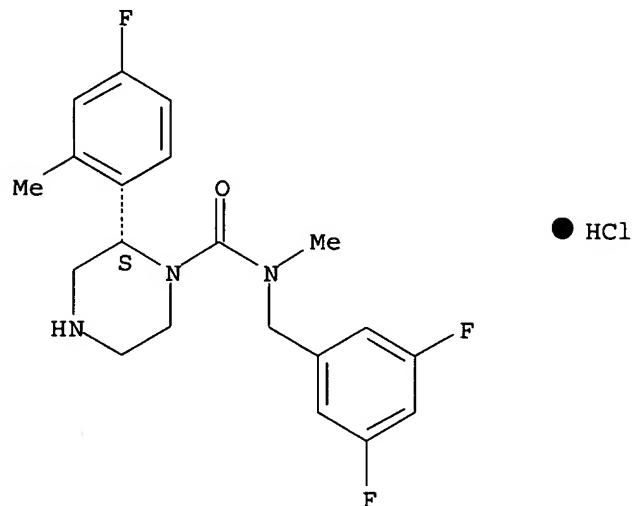
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10/089964

L2 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 470692-04-7 REGISTRY
CN 1-Piperazinecarboxamide, N-[(3,5-difluorophenyl)methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)
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MF C20 H22 F3 N3 O . Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (470692-12-7)

Absolute stereochemistry.

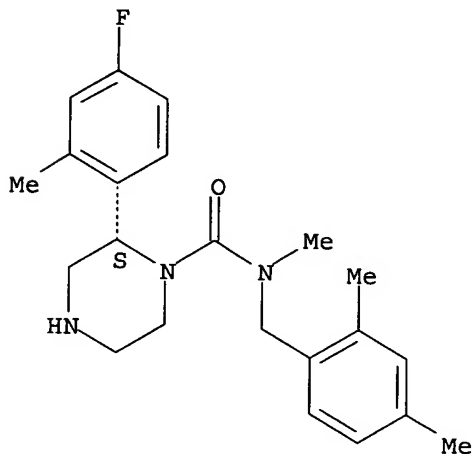


1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

10/089964

L2 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 470691-98-6 REGISTRY
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LC STN Files: CA, CAPLUS

Absolute stereochemistry.



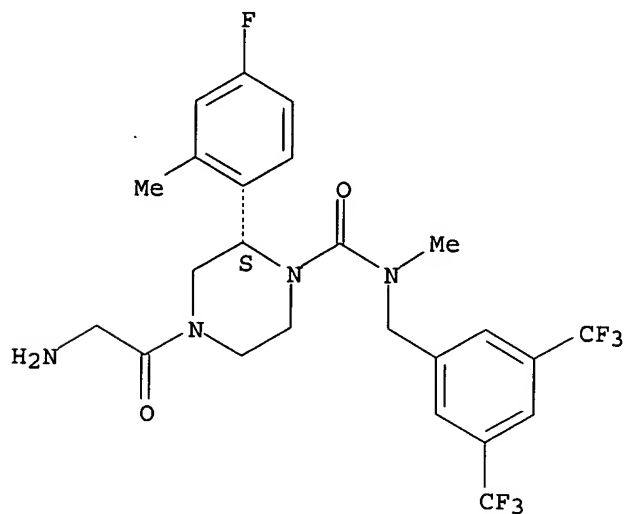
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

10/089964

L2 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 334476-75-4 REGISTRY
CN 1-Piperazinecarboxamide, 4-(aminoacetyl)-N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-2-(4-fluoro-2-methylphenyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
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CI COM
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

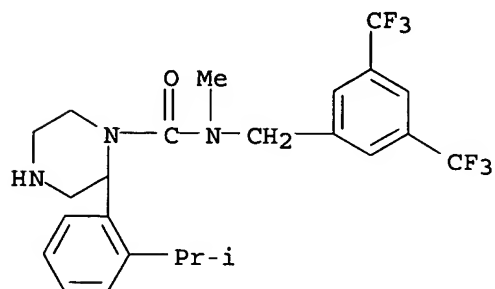


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

10/089964

L2 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 334476-65-2 REGISTRY
CN 1-Piperazinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-2-[2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)
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SR CA
LC STN Files: CA, CAPLUS, USPATFULL



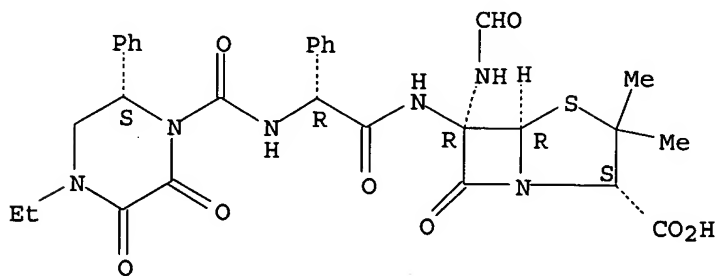
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

10/089964

L2 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2003 ACS
RN 123410-08-2 REGISTRY
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(4-ethyl-2,3-dioxo-2-phenyl-1-piperazinyl)carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.[S*(R*)]]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H32 N6 O8 S
CI .COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)